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function analyse_errors_bins(pos_estimated,score,pos, endbulges)
%analyse_errors_bins(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
if length(pos_estimated) ~= length(score)
    error('pos_estimated and score not compatible');
end
if length(pos_estimated) ~= length(pos)
    error('pos_estimated and pos not compatible');
end
if length(pos_estimated) ~= length(endbulges)
    error('pos_estimated and endbulges size not compatible');
end
N = 100;
Per_bin = 20;
mxscore = max(score);
mnscore = min(score);
dth = (mxscore- mnscore)/N;
thresh = mnscore:dth:mxscore;
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)-Per_bin
    I = find(score >= thresh(i) & score <= thresh(i+Per_bin));
    if ~isempty(I)
        count = count + 1;
        midbin(count) = 0.5*(thresh(i) + thresh(i+Per_bin));
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 2);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
    end
end

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midbin(count) = 0.25*(thresh(i) + 2* thresh(i+1) + thresh(i+2));
accuracy(count) = NaN;
correct_side_dist1(count) = NaN;
correct_side_dist2(count) = NaN;
correct_side_dsth(count) = NaN;
wrong_side(count) = NaN;
fraction(count) = NaN;
end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
clf
hold on

plot(midbin, acc2,'g')
plot(midbin, acc1,'r')
plot(midbin, accuracy,'b')
plot(midbin, wrong_side,'k')
plot(midbin,fraction,'c')

legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side');
plot(midbin, acc2,'*g')
plot(midbin, acc1,'or')
plot(midbin, accuracy,'bd')
plot(midbin, wrong_side,'kv')
xlabel('bin');
%keyboard
returnfunction analyse_errors_bins1(pos_estimated,score,pos, endbulges,N)
%analyse_errors_bins1(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
if length(pos_estimated) ~= length(score)
    error('pos_estimated and score not compatible');
end
if length(pos_estimated) ~= length(pos)
    error('pos_estimated and pos not compatible');
end
if length(pos_estimated) ~= length(endbulges)
    error('pos_estimated and endbulges size not compatible');
end
if nargin == 4
    N = 6;
end
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);

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fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1)))); %one for correct side estimate
end
for i = 1:length(thresh)-1
    I = find(score <= thresh(i) & score >= thresh(i+1));
    if ~isempty(I)
        count = count + 1;
        midbin(count) = mean(score(I));
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 2);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
        midbin(count) = NaN;;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
        correct_side_dsth(count) = NaN;
        wrong_side(count) = NaN;
        fraction(count) = NaN;
    end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
clf
hold on

plot(midbin, acc2,'g')
plot(midbin, acc1,'r')
plot(midbin, accuracy,'b')
plot(midbin, wrong_side,'k')
plot(midbin,fraction,'c')

legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side');
plot(midbin, acc2,'*g')

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plot(midbin, acc1,'or')
plot(midbin, accuracy,'bd')
plot(midbin, wrong_side,'kv')
xlabel('bin');
%keyboard
returnfunction analyse_errors_perc(pos_estimated,score,pos, endbulges)
%analyse_errors_perc(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
N = 100;
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)
    I = find(score > thresh(i));
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 2);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
        correct_side_dsth(count) = NaN;
        wrong_side(count) = NaN;
        fraction(count) = NaN;
    end
end
end

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acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
clf
hold on

plot(perc, acc2,'g')
plot(perc, acc1,'r')
plot(perc, accuracy,'b')
plot(perc, wrong_side,'k')
plot(perc, thresh,'c')
legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'threshold');
xlabel('percentage');
axis([0 100 0 1]);
%keyboard
returnfunction analyse_errors_thresh(pos_estimated,score,pos, endbulges)
%analyse_errors_thresh(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
if max(score) > 1
    mxscore = max(score);
else
    mxscore = 1;
end
if min(score) < 0
    mnscore = min(score);
else
    mnscore = 0;
end
Np = 500;
dth = (mxscore- mnscore)/Np;
thresh = mnscore:dth:mxscore;
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_disth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)
    I = find(score > thresh(i));
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);

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correct_side_dist1(count) = length(J1)/length(I);
J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
correct_side_dist2(count) = length(J2)/length(I);
Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 2);
correct_side_disth(count) = length(Jh)/length(I);

wrong_side(count) = sum(1-correct_side(I))/length(I);

fraction(count) = length(I)/N;
else
    count = count+1;
    accuracy(count) = NaN;
    correct_side_dist1(count) = NaN;
    correct_side_dist2(count) = NaN;
    correct_side_disth(count) = NaN;
    wrong_side(count) = NaN;
    fraction(count) = NaN;
end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
clf
hold on

plot(thresh, acc2,'g')
plot(thresh, acc1,'r')
plot(thresh, accuracy,'b')
plot(thresh, wrong_side,'k')
plot(thresh, fraction,'c')
legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'fraction');
xlabel('threshold');
%keyboard
returnfunction y = edit_distance(s,t)
% y = edit_distance(s,t)
% compute edit (levenstein) distance between s and t
C = 0.5; % parameter that fixes the relative
%Algorithm
%
%Construct a matrix containing 0..m rows and 0..n columns.
% Initialize the first row to 0..n.
% Initialize the first column to 0..m.
% 3. Examine each character of s (i from 1 to n).
% 4. Examine each character of t (j from 1 to m).
% 5. If s[i] equals t[j], the cost is 0.
%6. If s[i] doesn't equal t[j], the cost is 1.
% Set cell d[i,j] of the matrix equal to the minimum of:
%a. The cell immediately above plus 1: d[i-1,j] + 1.
%b. The cell immediately to the left plus 1: d[i,j-1] + 1.

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%c. The cell diagonally above and to the left plus the cost: d[i-1,j-1] + cost.
%7 After the iteration steps (3, 4, 5, 6) are complete, the distance is found in cell d[n,m]
n = length(s);
m = length(t);
if n == 0
    y = m;
    return;
end
if m == 0
    y = n;
    return;
end
d = zeros(n+1,m+1); %Construct a matrix containing 0..m rows and 0..n columns.
d(1,:) = [0:m];      % Initialize the first row to 0..n.
d(:,1) = [0:n]';     %Initialize the first column to 0..m.
for i = 1:n
    for j = 1:m
        cost = (s(i) ~= t(j));
        d(i+1,j+1) = min([d(i+1,j)+1, d(i,j+1)+1, d(i,j)+cost]);
    end
end
y = d(n+1,m+1);
return

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function [pos,score] = edit_predict(seqsd, seqs, endbulges)
% y = edit_predict(seqsd, seqs, endbulges)
% find the best matching dicer position by its edit distance to one of the existing dicers
%
% GD 20.2
global Min_dlength Alpha Step
paramfile = 'edit_params';
%addpath('d:/matlab'); % whereabouts of edit_distance
disp('calculating...');
Step = 1;
fid = fopen(paramfile,'r');
while ~feof(fid)
    line = fgetl(fid);
    eval(line)
end
fclose(fid);
for i = 1:length(seqs)
    %disp(num2str(i));
    [posi, scorei] = edit_predict1(seqsd,seqs{i}, endbulges{i});
    pos(i) = posi;
    score(i) = scorei;
end
return
function [pos, score] = edit_predict1(seqsd,seqsi, endbulgesi);
%calculate the best matching position of dicer
global Min_dlength Alpha Step

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seq_size = length(seqsi);
lb = find(endbulgesi);
eb_size = length(lb);
eb_begin = lb(1);
eb_end = lb(eb_size);
nd = length(seqsd); % number of known dicers
length_seqi = length(seqsi);
%initialize variables with the largest possible distance
min_d = ones(length_seqi,1)*Min_dlength;
mean_d = ones(length_seqi,1)*Min_dlength;
%upper side
for i = eb_begin-Min_dlength:-Step:1
    p = seqsi(i:i+Min_dlength-1);
    for j = 1:length(seqsd)
        % d(j) = edit_distance(p,seqsd{j});
        d(j) = editD(p,seqsd{j});
    %    d(j) = editD(p,seqsd{j});
    end
    min_d(i) = min(d);
    % take also the mean of highest percentile
    [ds,I] = sort(d);
    mean_d(i) = mean(ds(1:floor(Alpha*nd)));
end
for i = eb_end+1:Step:length(seqsi)-Min_dlength+1
    p = seqsi(i:i+Min_dlength-1);
    for j = 1:length(seqsd)
        d(j) = editD(p,seqsd{j});
    end
    min_d(i) = min(d);
    % take also the mean of highest ten percentile
    [ds,I] = sort(d);
    mean_d(i) = mean(ds(1:floor(Alpha*nd)));
end
mmn = min(min_d);
I = find(min_d == mmn);
if length(I) == 1
    pos = I;
    score = Min_dlength - mmn;
else
    % take the position with hte highest alpha score
    [mn,J] = min(mean_d(I));
    pos = I(J);
    score = Min_dlength - mmn;
end
return
function [pos,score] = edit_predictk(seqsd, seqs, endbulges, k, thresh)
% y = edit_predictk(seqsd, seqs, endbulges, k, thresh);
% find the best matching dicer position by its edit distance to one of the existing dicers
% criterion is mean among best k matches
%thresh is the

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% GD 20.2
global Min_dlength Step
paramfile = 'edit_params';
addpath('d:/matlab'); % whereabouts of edit_distance
if nargin <= 4
    thresh = 1.1;
end
if length(seqs) ~= length(endbulges)
    error('size of seqs and endbulges not compatible');
end
if thresh < 1
    error('thresh must be < 1');
end
Step = 1;
fid = fopen(paramfile,'r');
while ~feof(fid)
    line = fgetl(fid);
    eval(line)
end
fclose(fid);
for i = 1:length(seqs)
    disp(num2str(i));
    [posi, scorei] = edit_predict1(seqsd,seqs{i}, endbulges{i},k,thresh);
    pos(i) = posi;
    score(i) = scorei;
end
return
function [pos, score] = edit_predict1(seqsd,seqsi, endbulgesi,k,thresh);
%calculate the best matching position of dicer
global Min_dlength Step
seq_size = length(seqsi);
lb = find(endbulgesi);
eb_size = length(lb);
eb_begin = lb(1);
eb_end = lb(eb_size);
nd = length(seqsd); % number of known dicers
length_seqi = length(seqsi);
%initialize variables with the largest possible distance
min_d = ones(length_seqi,1)*Min_dlength;
mean_d = ones(length_seqi,1)*Min_dlength;
%upper side
for i = eb_begin-Min_dlength:-Step:1
    p = seqsi(i:i+Min_dlength-1);
    for j = 1:length(seqsd)
        d(j) = edit_distance(p,seqsd{j});
    end
    % take also the mean of best k
    [ds,l] = sort(d);
    mean_d(i) = mean(ds(1:k));
end
end

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%lower side
for i = eb_end+1:Step:length(seqsi)-Min_dlength+1
    p = seqsi(i:i+Min_dlength-1);
    for j = 1:length(seqsd)
        d(j) = edit_distance(p,seqsd{j});
    end
    [ds,l] = sort(d);
    mean_d(i) = mean(ds(1:k));
end
mmn = min(mean_d);
l = find(mean_d <= thresh* mmn);
if length(l) ==1
    pos = l;
    score = Min_dlength - mmn;
else
    % take the position closest to loop
    side = sign(l - eb_begin);
    loopdist = 0.5*(1-side).* (eb_begin - l - Min_dlength) + 0.5*(1+side).*(l- eb_end-1);
    [mndist,J] = min(loopdist);
    l = l(J);
    pos = l;
    score = Min_dlength - mean_d(l);
end
return
function [si,sj] = find_identical_pairs(seqs)
%[si,sj] = find_identical_pairs(seqs)
% find identical palindromes in list
L = length(seqs);
for i = 1:L
    lenp(i) = length(seqs{i});
end
[lenps, l] = sort(lenp);
seqs = seqs(l);
count = 0;
for i = 1:L
    for j = i+1:L
        if lenps(i) ~= lenps(j)
            break
        else
            if all(seqs{i} == seqs{j})
                count = count+1;
                si(count) = l(i);
                sj(count) = l(j);
            end
        end
    end
end
end
end

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function strseq = int2nuc(intseq, ncase)
%strseq = int2nuc(intseq, ncase)

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%convert a sequence of '1 2 3 4' into 'A C T G' or 'a c t g'
% ncase = uppercase | lowercase
if nargin == 1
    ncase = 'uppercase';
end
if strcmp(ncase,'uppercase')
    nucs = 'ACTG';
elseif strcmp(ncase,'lowercase')
    nucs = 'actg';
end
strseq = char(size(intseq));
for i = 1:length(intseq)
    strseq(i) = nucs(intseq(i));
end
return
method = 'poly3'
if method == 'poly2'
% poly2 combined
    %configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    %points on side error line
    as = [-1.5000 -0.9988 -0.5012 -0.0035 0.5012 0.99 1.4927];
    bs = [0.2325 0.2295 0.1360 0.0804 0.0336 0.0102 0.0015];
    %points on precise within2 line
    ap = [-1.4965 -0.9988 -0.5012 0.0035 0.5012 0.9988];
    bp = [0.6798 0.6974 0.8348 0.9196 0.9722 0.9985];
elseif method == 'poly3'
    % configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    % alpha5 = 0.9; alpha3 = 0.40; alpha_dlen = 0.2;
    %points on side error line
    as = [-1.4981 -1.2412 -0.9994 -0.5006 0.0019 0.5044 0.7727 0.9994 1.2714 1.5057];
    bs = [0.2303 0.2248 0.2028 0.1239 0.0872 0.0560 0.0211 0.0211 0 0];
    %points on precise within2 line
    ap = [-1.4981 -1.3281 -1.0031 -0.4931 0.0019 0.4969 0.9994 1.5000];
    bp = [0.6940 0.7000 0.7312 0.8688 0.9165 0.9404 0.9752 1.0000
yside = 1-interp1(as,bs,xi,'linear','extrap')
yprec = interp1(ap,bp,xi,'linear','extrap')
function [yside, yprec2] = interpolate_prob_new(score, fitfile);
%[yside, yprec2] = interpolate_prob_new(score, fitfile);
% load the parameters for interpolation
fid = fopen(fitfile,'r');
while ~feof(fid)
    line = fgetl(fid);
    if ~isstr(line), break , end;
    eval(line)
end
fclose(fid);
%interpolate
yside = interp1(xs,ys,score,'linear');
yprec2 = interp1(xp2,yp2,score,'linear');
returnfunction [yside, yprec2] = interpolate_prob_old_ver5(xi, method);

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%[yside, yprec2] = interpolate_prob_old_ver5(yi, method);
% parameters are configuration specific see below!
disp('these are the accumulated performance, not the actual performance per bin');
disp(' press enter to continue');
pause
if nargin == 1
    method = 'poly3';
end
if strcmp(method, 'poly2')
% poly2 combined
    %configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    %points on side error line
    as = [-1.5000 -0.9988 -0.5012 -0.0035 0.5012 0.99 1.4927];
    bs = [0.2325 0.2295 0.1360 0.0804 0.0336 0.0102 0.0015];
%points on precise within2 line
    ap = [-1.4965 -0.9988 -0.5012 0.0035 0.5012 0.9988];
    bp = [0.6798 0.6974 0.8348 0.9196 0.9722 0.9985];
elseif strcmp(method, 'poly3')
    % configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    % alpha5 = 0.9; alpha3 = 0.40; alpha_dlen = 0.2;
    %points on side error line
    as = [-1.4981 -1.2412 -0.9994 -0.5006 0.0019 0.5044 0.7727 0.9994 1.2714 1.5057];
    bs = [0.2303 0.2248 0.2028 0.1239 0.0872 0.0560 0.0211 0.0211 0 0];
    %points on precise within2 line
    ap = [-1.4981 -1.3281 -1.0031 -0.4931 0.0019 0.4969 0.9994 1.5000];
    bp = [0.6940 0.7000 0.7312 0.8688 0.9165 0.9404 0.9752 1.0000];
end
yside = 1-interp1(as,bs,xi,'linear');
yprec2 = interp1(ap,bp,xi,'linear');
function [yside, yprec2] = interpolate_probabilities(xi, method);
%[yside, yprec2] = interpolate_probabilities(yi, method);
% parameters are configuration specific see below!
if nargin == 1
    method = 'poly3';
end
if strcmp(method, 'poly3')
    % configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    % alpha5 = 0.9; alpha3 = 0.40; alpha_dlen = 0.2;
    %points on side error line
    as = [1.5000 1.3235 1.2591 0.9478 0.2052 -0.1707 -0.3337 -0.5573 -0.7706 -1.0873];
    bs = [1.0000 1.0000 0.9355 0.8710 0.8485 0.8438 0.8182 0.5806 0.5000 0.5000];
    ap = as;
    bp = [1.0000 1.0000 0.9355 0.8710 0.8485 0.8438 0.7576 0.4839 0.2803 0.2681];
end
yside = 1-interp1(as,bs,xi,'linear','extrap');
yprec2 = interp1(ap,bp,xi,'linear','extrap');
function [yside, yprec2] = interpolate_probabilities_ver5(xi, method);
%[yside, yprec2] = interpolate_probabilities_ver5(yi, method);
% parameters are configuration specific see below!
disp('these are the accumulated performance, not the actual performance per bin');

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```

disp(' press enter to continue');
pause
if nargin == 1
    method = 'poly3';
end
if strcmp(method, 'poly2')
% poly2 combined
    %configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    %points on side error line
    as = [-1.5000 -0.9988 -0.5012 -0.0035 0.5012 0.99 1.4927];
    bs = [0.2325 0.2295 0.1360 0.0804 0.0336 0.0102 0.0015];
%points on precise within2 line
    ap = [-1.4965 -0.9988 -0.5012 0.0035 0.5012 0.9988];
    bp = [0.6798 0.6974 0.8348 0.9196 0.9722 0.9985];
elseif strcmp(method, 'poly3')
    % configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    % alpha5 = 0.9; alpha3 = 0.40; alpha_dlen = 0.2;
    %points on side error line
    as = [-1.4981 -1.2412 -0.9994 -0.5006 0.0019 0.5044 0.7727 0.9994 1.2714 1.5057];
    bs = [0.2303 0.2248 0.2028 0.1239 0.0872 0.0560 0.0211 0.0211 0 0];
    %points on precise within2 line
    ap = [-1.4981 -1.3281 -1.0031 -0.4931 0.0019 0.4969 0.9994 1.5000];
    bp = [0.6940 0.7000 0.7312 0.8688 0.9165 0.9404 0.9752 1.0000];
end
yside = 1-interp1(as,bs,xi,'linear');
yprec2 = interp1(ap,bp,xi,'linear');
function [yside, yprec2] = interpolate_probabilities_ver5(xi, method);
%[yside, yprec2] = interpolate_probabilities_ver5(yi, method);
% parameters are configuration specific see below!
disp('these are the accumulated performance, not the actual performance per bin');
disp(' press enter to continue');
pause
if nargin == 1
    method = 'poly3';
end
if strcmp(method, 'poly2')
% poly2 combined
    %configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    %points on side error line
    as = [-1.5000 -0.9988 -0.5012 -0.0035 0.5012 0.99 1.4927];
    bs = [0.2325 0.2295 0.1360 0.0804 0.0336 0.0102 0.0015];
%points on precise within2 line
    ap = [-1.4965 -0.9988 -0.5012 0.0035 0.5012 0.9988];
    bp = [0.6798 0.6974 0.8348 0.9196 0.9722 0.9985];
elseif strcmp(method, 'poly3')
    % configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    % alpha5 = 0.9; alpha3 = 0.40; alpha_dlen = 0.2;
    %points on side error line
    as = [-1.4981 -1.2412 -0.9994 -0.5006 0.0019 0.5044 0.7727 0.9994 1.2714 1.5057];
    bs = [0.2303 0.2248 0.2028 0.1239 0.0872 0.0560 0.0211 0.0211 0 0];

```

```

%points on precise within2 line
ap = [-1.4981 -1.3281 -1.0031 -0.4931 0.0019 0.4969 0.9994 1.5000];
bp = [0.6940 0.7000 0.7312 0.8688 0.9165 0.9404 0.9752 1.0000];
end
yside = 1-interp1(as,bs,xi,'linear');
yprec2 = interp1(ap,bp,xi,'linear');
function [yside, yprec2] = interpolate_probabilities_ver5(xi, method);
%[yside, yprec2] = interpolate_probabilities_ver5(yi, method);
% parameters are configuration specific see below!
disp('version 5 does not allow for extrapolation')
if nargin == 1
    method = 'poly3';
end
if strcmp(method,'poly3')
    % configuration: 5' -2 7 -2 6 3' -11 0 -11 0
    % alpha5 = 0.9; alpha3 = 0.40; alpha_dlen = 0.2;
    %points on side error line
    as = [1.5000 1.3235 1.2591 0.9478 0.2052 -0.1707 -0.3337 -0.5573 -0.7706 -1.0873];
    bs = [1.0000 1.0000 0.9355 0.8710 0.8485 0.8438 0.8182 0.5806 0.5000 0.5000];
    ap = as;
    bp = [1.0000 1.0000 0.9355 0.8710 0.8485 0.8438 0.7576 0.4839 0.2803 0.2681];
end
%yside = 1-interp1(as,bs,xi,'linear','extrap');
%yprec2 = interp1(ap,bp,xi,'linear','extrap');
yside = 1-interp1(as,bs,xi,'linear');
yprec2 = interp1(ap,bp,xi,'linear');
function len = length_seq(seqs);
%len = length_seq(seqs);
%calculate sequence length
for i = 1:length(seqs)
    len(i) = length(seqs{i});
end
returnl = find(lenp-pos >= 22);
for i = 1:length(l)
    frstl(i) = seqs{l(i)}(pos(l(i)));
    lastl(i,:) = seqs{l(i)}([20+pos(l(i)), 21+pos(l(i))]);
end %load training data
randomize = 1;
curdir = pwd;
cd d:/rosetta/data_new
load matlab_147_unique.mat
if randomize
    disp('performing randomized permutation');
    l = randperm(length(seqs));
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    endbulges = endbulges(l);
    lend = lend(l);
    lenp = lenp(l);
    pos = pos(l);

```

```

seq_id = seq_id(l);
seqs = seqs(l);
seqsd = seqsd(l);
end
cd(curdir) %load training data
randomize = 0;
curdir = pwd;
cd d:/rosetta/data_new
load matlab_147_unique.mat
if randomize
    disp('performing randomized permutation');
    l = randperm(length(seqs));
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    endbulges = endbulges(l);
    lend = lend(l);
    lenp = lenp(l);
    pos = pos(l);
    seq_id = seq_id(l);
    seqs = seqs(l);
    seqsd = seqsd(l);
end
cd(curdir) %load training data
curdir = pwd;
cd d:/rosetta/data_new
load matlab_173_unique.mat
cd(curdir) function pos = locate_dicer(dicer_seq,pal_seq);
%pos = locate_dicer(dicer_seq,palseq)
%get absolute position of dicer on palindrom, from the beginning of the plindrom
if length(dicer_seq) ~= length(pal_seq)
    error('different number of sequences');
end
pos = zeros(1,length(dicer_seq));
for i = 1:length(dicer_seq)
    l = findstr(dicer_seq{i}, pal_seq{i});
    if length(l) == 1
        pos(i) = l;
    else
        pos(i) = NaN;
    end
end
end
function pos_dummy = make_pos_dummy(seqs,bulges1,bulges2,endbulges)
%pos_dummy = make_pos_dummy(seqs,bulges1,bulges2,endbulges)
% construct dummy pos vector for testing classifiers
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
mode = 'testing'
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
pos_dummy = zeros(1, length(seqs));
for i = 1:length(seqs)

```

```

    pos_dummy(i) = mkpsi0(seqs{i},bulges1{i},bulges2{i},endbulges{i});
    %pos_dummy(i) = mkpsi1(seqs{i},bulges1{i},bulges2{i},endbulges{i});
end
return
% version 0
function posi = mkpsi0(seqs,i,bulges2i,endbulgesi)
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
% simple rule
% assume dicer of length 17 exactly.
% nearest , in euclidean distance to some prototype, regardless of distance
% from loop and side
% params are assumed -2 3 -2 7
prototype = [0.3381,-0.4804,0.1813,-0.1205,0.3318,0.0028,0.2095,-0.3635, ...
-0.0711,-0.1954,-0.3103,-0.3066,0.1822,-0.1972,0.0417,0.3385,-0.4882, ...
-0.3491,0.1979,-0.1216,0.3600,0.3537,0.0936,0.2271,-0.1907,0.3939, ...
0.3385,0.0681,-0.1296,0.2027,0.0466,0.2948,0.4568,0.0226,0.0182,...
0.0828,-0.0765,0.0155,-0.1660,-0.0671,-0.2741,0.0798,-0.3252,0.0678 ...
0.2604,0.0298,0.1405,-0.2909,-0.1202,0.2833,0.1808,-0.4104,-0.0389];
seq_size = length(seqs);
lb = find(endbulgesi);
eb_size = length(lb);
eb_begin = lb(1);
[xi, yi] = preprocess5(seqs,i,bulges2i,endbulgesi);
[m,n] = size(xi);
sim = xi(:,3:n)*(prototype(1:n-2))';
[maxs,m] = max(sim);
side = xi(m,1);
loopdist = xi(m,2) * (0.5* (seq_size - eb_size));
posi = (1+side)/2*(eb_end + loopdist) + (1-side)/2*(eb_begin - loopdist);
return
% version 1
function posi = mkpsi1(seqs,i,bulges2i,endbulgesi)
% simple rule
% assume dicer of length 17 exactly.
% nearest position to loop, such that dicer begins with t , not on bulge1
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
lb = find(endbulgesi);
eb_size = length(lb);
eb_begin = lb(1);
eb_end = lb(eb_size);
pos = find(seqs == 3 & endbulgesi == 0 & bulges1i == 0);
dst = zeros(size(pos));
if ~isempty(pos)
    side = sign(pos-eb_begin);
    lup = find(side == -1);
    dst(lup) = eb_begin - (pos(lup) + Min_dlength - 1);
    ldwn = find(side == 1);
    dst(ldwn) = pos(ldwn) - eb_end;
end

```

```

    dst(find(dst < 0))= 1000;
    [md,l] = min(dst);
    posi = pos(l);
else
    pos = find(seqsi == 4 & endbulgesi == 0 & bulges1i == 0);
    side = sign(pos-eb_begin);
    lup = find(side == -1);
    dst(lup) = eb_begin - (pos(lup) + Min_dlength -1);
    ldwn = find(side == 1);
    dst(ldwn) = pos(ldwn) - eb_end;
    on_endbulge = find(dst < 0);
    dst(on_endbulge) == 1000;
    [md,l] = min(dst);
    posi = pos(l);
end
return
function [x,y,seqno] = merge_sets(x1,x2,y1,y2,seqno1,seqno2)
%[x,y,seqno] = merge_sets(x1,x2,y1,y2,seqno1,seqno2)
% concatenate datasets
x = [x1; x2];
y = [y1; y2];
seqno = [seqno1; seqno2+max(seqno1)];
return%mfold_cv
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
pos5 = zeros(0);
score5 =zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];% test set
    bt = setdiff(bins_all , bs);% train set

    disp(' ');
    disp(['m = ' num2str(m)]);

    [pos5m,score5m] = edit_predict(seqsd(bt), seqs(bs), endbulges(bs));

    pos5 = [pos5,pos5m];
    score5 =[score5,score5m];

    m = m+1;
end
% perform m fold cross validation on article + zuker results by splitting set
validation = 1; % otherwise, only testing is performed
mfold = 5;
n_all = 278;
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;

```

```

x3 = zeros(0);
out3 =zeros(0);
seqno3 = zeros(0);
pos3 = zeros(0);
score3 = zeros(0);
x5 = zeros(0);
out5 =zeros(0);
seqno5 = zeros(0);
pos5 = zeros(0);
score5 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
    % test set
    filename3 = ['svm_tst_3m.dat'];
    filename5 = ['svm_tst_5m.dat'];
    [x3s, seqno3s] = preprocess_and_write_data3(seqs_all(bs),bulges1_all(bs),bulges2_all(bs),endbulges_all(bs),
filename3);
    [x5s, seqno5s] = preprocess_and_write_data5(seqs_all(bs),bulges1_all(bs),bulges2_all(bs),endbulges_all(bs),
filename5);
    disp(['m = ' num2str(m)]);
    disp('written preprocessed test examples');

    bt = setdiff(bins_all , bs);
    filename3 = ['svm_trn_3m.dat'];
    filename5 = ['svm_trn_5m.dat'];
    [x3t, seqno3t] = preprocess_and_write_data3(seqs_all(bt),bulges1_all(bt),bulges2_all(bt),endbulges_all(bt),
filename3, pos_all(bt)+lend_all(bt)-1);
    [x5t, seqno5t] = preprocess_and_write_data5(seqs_all(bt),bulges1_all(bt),bulges2_all(bt),endbulges_all(bt),
filename5, pos_all(bt));
    disp('written preprocessed training examples');

    disp('now train and test svm. results should be in g:\research\rosetta\svm_light_utils1\svm_outputs\out3m.out,
out5m.out');
    disp('*****');

    pause
    cd svm_outputs
    load out3m.out
    load out5m.out
    cd ..
    [pos3m, score3m] = svm_position(x3s,out3m,seqno3s, endbulges_all(bs), lenp_all(bs)+lend_all(bs));
    [pos5m, score5m] = svm_position(x5s,out5m,seqno5s, endbulges_all(bs), lenp_all(bs));
    %collect global variables
    x3 = [x3; x3s];
    out3 =[out3;out3m];
    if m == 1
        seqno3 = seqno3s;
    else
        mx3 = max(seqno3);

```

```

    seqno3 = [seqno3 ; mx3+seqno3s];
end
pos3 = [pos3 pos3m];
score3 = [score3 score3m];

x5 = [x5;x5s];;
out5 =[out5;out5m];
if m == 1
    seqno5 = seqno5s;
else
    mx5 = max(seqno5);
    seqno5 = [seqno5 ; mx3+seqno5s];
end
pos5 = [pos5 pos5m];
score5 = [score5 score5m];
m = m+1;
end
%mfold_cv_transduction
% perform m fold cross validation on article + zucker results by splitting set
% use transduction mode of SVM
mfold = 5;
n_all = 278;
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
x3 = zeros(0);
out3 =zeros(0);
seqno3 = zeros(0);
pos3 = zeros(0);
score3 = zeros(0);
x5 = zeros(0);
out5 =zeros(0);
seqno5 = zeros(0);
pos5 = zeros(0);
score5 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1 : bins(m+1)];
    %training set
    bt = setdiff(bins_all , bs);
    filename3 = ['svm_trn_3t.dat'];
    filename5 = ['svm_trn_5t.dat'];
    [x3t, seqno3t] = preprocess_and_write_data3(seqs_all(bt),bulges1_all(bt),bulges2_all(bt),endbulges_all(bt),
    filename3, pos_all(bt)+lend_all(bt)-1);
    [x5t, seqno5t] = preprocess_and_write_data5(seqs_all(bt),bulges1_all(bt),bulges2_all(bt),endbulges_all(bt),
    filename5, pos_all(bt));
    disp('written preprocessed training examples');

% test set - append to previous file
    [x3s, seqno3s] = preprocess_and_write_data3_tr(seqs_all(bs),bulges1_all(bs),bulges2_all(bs),endbulges_all(bs),
    filename3);

```

```
[x5s, seqno5s] = preprocess_and_write_data5_tr(seqs_all(bs),bulges1_all(bs),bulges2_all(bs),endbulges_all(bs),
filename5);
```

```
% test set - write to seperate file
filename3 = ['svm_tst_3t.dat'];
filename5 = ['svm_tst_5t.dat'];
[x3s, seqno3s] = preprocess_and_write_data3(seqs_all(bs),bulges1_all(bs),bulges2_all(bs),endbulges_all(bs),
filename3);
[x5s, seqno5s] = preprocess_and_write_data5(seqs_all(bs),bulges1_all(bs),bulges2_all(bs),endbulges_all(bs),
filename5);
disp('written preprocessed testing examples');
disp(['m = ' num2str(m)]);
disp('written preprocessed test examples');
```

```
disp('now train and test svm. ');
disp('transductive data are in svm_trn_5t.dat etc.')
disp('results should be in g:\research\rosetta\svm_light_utils1\svm_outputs\out5t.out, etc. ');
disp('*****');
```

```
pause
cd svm_outputs
load out3t.out
load out5t.out
cd ..
[pos3t, score3t] = svm_position(x3s,out3t,seqno3s, endbulges_all(bs), lenp_all(bs)+lend_all(bs));
[pos5t, score5t] = svm_position(x5s,out5t,seqno5s, endbulges_all(bs), lenp_all(bs));
%collect global variables
x3 = [x3; x3s];
out3 =[out3;out3t];
if m == 1
    seqno3 = seqno3s;
else
    mx3 = max(seqno3);
    seqno3 = [seqno3 ; mx3+seqno3s];
end
pos3 = [pos3 pos3t];
score3 = [score3 score3t];
```

```
%here am
```

```
x5 = [x5;x5s];;
out5 =[out5;out5t];
if m == 1
    seqno5 = seqno5s;
else
    mx5 = max(seqno5);
    seqno5 = [seqno5 ; mx3+seqno5s];
end
pos5 = [pos5 pos5t];
```



```

score5 = [score5 score5t];
m = m+1;
end
% perform m fold cross validation on article + zucker results by splitting set
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
svm_params = input('enter svm parameters: ','s');
model_filename3 = 'd:/svm_light/model3m';
tst_filename3 = 'd:/rosetta/svm_light_utils1/svm_tst_3m.dat';
trn_filename3 = 'd:/rosetta/svm_light_utils1/svm_trn_3m.dat';
out_filename3 = 'd:/rosetta/svm_light_utils1/out3m.out';
x3 = zeros(0);
out3 = zeros(0);
seqno3 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
    % test set

[x3s, seqno3s] = preprocess_and_write_data3(seqs(bs),bulges1(bs), ...
    bulges2(bs),endbulges(bs), tst_filename3);
    disp(['m = ' num2str(m)]);
    disp('written preprocessed test examples');

    bt = setdiff(bins_all , bs);

    [x3t, seqno3t] = preprocess_and_write_data3(seqs(bt),bulges1(bt),...
        bulges2(bt),endbulges(bt), trn_filename3, pos(bt)+lend(bt)-1);
    disp('written preprocessed training examples');

dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename3 ' ' model_filename3]);
dos(['d:/svm_light/svm_classify ' tst_filename3 ' ' model_filename3 ' ' out_filename3]);

load out3m.out

%collect global variables
x3 = [x3;x3s];
out3 =[out3;out3m];
if m == 1
    seqno3 = seqno3s;
else
    mx3 = max(seqno3);
    seqno3 = [seqno3 ; mx3+seqno3s];
end
m = m+1;
end
clear x3s x3t out3m seqno3s seqno3t bs bt
% just for printing the info

```

```

[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params3.dat');
disp(' ');
disp('*****');
disp('3 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) '']);
disp(['svm light params: ' svm_params]);
% perform m fold cross validation on article + zucker results by splitting set
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
svm_params = input('enter svm parameters: ','s');
model_filename3 = 'd:/svm_light/model3m';
tst_filename3 = 'd:/rosetta/svm_light_utils1/svm_tst_3mb.dat';
trn_filename3 = 'd:/rosetta/svm_light_utils1/svm_trn_3mb.dat';
out_filename3 = 'd:/rosetta/svm_light_utils1/out3mb.out';
x3 = zeros(0);
out3 = zeros(0);
seqno3 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
    % test set

[x3s, seqno3s] = preprocess_and_write_data3(seqs(bs),bulges1(bs), ...
    bulges2(bs),endbulges(bs), tst_filename3);
    disp(['m = ' num2str(m)]);
    disp('written preprocessed test examples');

    bt = setdiff(bins_all , bs);

[x3t, seqno3t] = preprocess_and_write_data3(seqs(bt),bulges1(bt),...
    bulges2(bt),endbulges(bt), trn_filename3, pos(bt)+lend(bt)-1);
    disp('written preprocessed training examples');

dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename3 ' ' model_filename3]);
dos(['d:/svm_light/svm_classify ' tst_filename3 ' ' model_filename3 ' ' out_filename3]);

load out3mb.out
out3m= out3mb;

%collect global variables
x3 = [x3;x3s];
out3 =[out3;out3m];
if m == 1
    seqno3 = seqno3s;
else
    mx3 = max(seqno3);
    seqno3 = [seqno3 ; mx3+seqno3s];
end

```

```

    m = m+1;
end
clear x3s x3t out3m out3mb seqno3s seqno3t bs bt
% just for printing the info
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params3.dat');
disp(' ');
disp('*****');
disp('3 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) ]);
disp(['svm light params: ' svm_params]);
% perform m fold cross validation on article + zucker results by splitting set
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
svm_params = input('enter svm parameters: ','s');
model_filename5 = 'd:/svm_light/model5m';
tst_filename5 = 'd:/rosetta/svm_light_utils1/svm_tst_5m.dat';
trn_filename5 = 'd:/rosetta/svm_light_utils1/svm_trn_5m.dat';
out_filename5 = 'd:/rosetta/svm_light_utils1/out5m.out';
x5 = zeros(0);
out5 = zeros(0);
seqno5 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
    % test set

[x5s, seqno5s] = preprocess_and_write_data5(seqs(bs),bulges1(bs), ...
    bulges2(bs),endbulges(bs), tst_filename5);
    disp(['m = ' num2str(m)]);
    disp('written preprocessed test examples');

    bt = setdiff(bins_all , bs);

[x5t, seqno5t] = preprocess_and_write_data5(seqs(bt),bulges1(bt),...
    bulges2(bt),endbulges(bt), trn_filename5, pos(bt));
    disp('written preprocessed training examples');

dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename5 ' ' model_filename5]);
dos(['d:/svm_light/svm_classify ' tst_filename5 ' ' model_filename5 ' ' out_filename5]);

load out5m.out

%collect global variables
x5 = [x5;x5s];
out5 =[out5;out5m];
if m == 1
    seqno5 = seqno5s;
else

```

```

mx5 = max(seqno5);
seqno5 = [seqno5 ; mx5+seqno5s];
end
m = m+1;
end
clear x5s x5t out5m seqno5s seqno5t bs bt
% just for printing the info
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
disp(' ');
disp('*****');
disp('5 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) ]);
disp(['svm light params: ' svm_params]);
% perform m fold cross validation on article + zucker results by splitting set
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
svm_params = input('enter svm parameters: ','s');
model_filename5 = 'd:/svm_light/model5m';
tst_filename5 = 'd:/rosetta/svm_light_utils1/svm_tst_5m.dat';
trn_filename5 = 'd:/rosetta/svm_light_utils1/svm_trn_5m.dat';
out_filename5 = 'd:/rosetta/svm_light_utils1/out5m.out';
model_filename3 = 'd:/svm_light/model3m';
tst_filename3 = 'd:/rosetta/svm_light_utils1/svm_tst_3m.dat';
trn_filename3 = 'd:/rosetta/svm_light_utils1/svm_trn_3m.dat';
out_filename3 = 'd:/rosetta/svm_light_utils1/out3m.out';
x3 = zeros(0);
out3 = zeros(0);
seqno3 = zeros(0);
pos3 = zeros(0);
score3 = zeros(0);
x5 = zeros(0);
out5 = zeros(0);
seqno5 = zeros(0);
pos5 = zeros(0);
score5 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
% test set
    [x3s, seqno3s] = preprocess_and_write_data3(seqs(bs),bulges1(bs),bulges2(bs),endbulges(bs), tst_filename3);
    [x5s, seqno5s] = preprocess_and_write_data5(seqs(bs),bulges1(bs),bulges2(bs),endbulges(bs), tst_filename5);
    disp(['m = ' num2str(m)]);
    disp('written preprocessed test examples');

    bt = setdiff(bins_all , bs);
    [x3t, seqno3t] = preprocess_and_write_data3(seqs(bt),bulges1(bt),bulges2(bt),endbulges(bt), trn_filename3,
pos(bt)+lend(bt)-1);
    [x5t, seqno5t] = preprocess_and_write_data5(seqs(bt),bulges1(bt),bulges2(bt),endbulges(bt), trn_filename5,
pos(bt));

```

```

disp('written preprocessed training examples');

dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename5 ' ' model_filename5]);
dos(['d:/svm_light/svm_classify ' tst_filename5 ' ' model_filename5 ' ' out_filename5]);
dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename3 ' ' model_filename3]);
dos(['d:/svm_light/svm_classify ' tst_filename3 ' ' model_filename3 ' ' out_filename3]);

load(out_filename3);
load(out_filename5)

%[pos3m, score3m] = svm_position(x3s,out3m,seqno3s, endbulges(bs), lenp(bs));
%[pos5m, score5m] = svm_position(x5s,out5m,seqno5s, endbulges(bs), lenp(bs));
%collect global variables
x3 = [x3; x3s];
out3 =[out3;out3m];
if m == 1
    seqno3 = seqno3s;
else
    mx3 = max(seqno3);
    seqno3 = [seqno3 ; mx3+seqno3s];
end
% pos3 = [pos3 pos3m];
% score3 = [score3 score3m];

x5 = [x5;x5s];;
out5 =[out5;out5m];
if m == 1
    seqno5 = seqno5s;
else
    mx5 = max(seqno5);
    seqno5 = [seqno5 ; mx3+seqno5s];
end
% pos5 = [pos5 pos5m];
% score5 = [score5 score5m];
m = m+1;
end
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
disp(' ');
disp('*****');
disp('5 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) ]);
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params3.dat');
disp(' ');
disp('*****');
disp('3 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) ]);
disp(['svm light params: ' svm_params]);% perform m fold cross validation on article + zucker results by splitting set
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)

```

```

bins_all = 1:n_all;
svm_params = input('enter svm parameters: ','s');
model_filename5 = 'd:/svm_light/model5mb';
tst_filename5 = 'd:/rosetta/svm_light_utils1/svm_tst_5mb.dat';
trn_filename5 = 'd:/rosetta/svm_light_utils1/svm_trn_5mb.dat';
out_filename5 = 'd:/rosetta/svm_light_utils1/out5mb.out';
model_filename3 = 'd:/svm_light/model3mb';
tst_filename3 = 'd:/rosetta/svm_light_utils1/svm_tst_3mb.dat';
trn_filename3 = 'd:/rosetta/svm_light_utils1/svm_trn_3mb.dat';
out_filename3 = 'd:/rosetta/svm_light_utils1/out3mb.out';
x3 = zeros(0);
out3 = zeros(0);
seqno3 = zeros(0);
pos3 = zeros(0);
score3 = zeros(0);
x5 = zeros(0);
out5 = zeros(0);
seqno5 = zeros(0);
pos5 = zeros(0);
score5 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
% test set
    [x3s, seqno3s] = preprocess_and_write_data3(seqs(bs),bulges1(bs),bulges2(bs),endbulges(bs), tst_filename3);
    [x5s, seqno5s] = preprocess_and_write_data5(seqs(bs),bulges1(bs),bulges2(bs),endbulges(bs), tst_filename5);
    disp(['m = ' num2str(m)]);
    disp('written preprocessed test examples');

    bt = setdiff(bins_all , bs);
    [x3t, seqno3t] = preprocess_and_write_data3(seqs(bt),bulges1(bt),bulges2(bt),endbulges(bt), trn_filename3,
pos(bt)+lend(bt)-1);
    [x5t, seqno5t] = preprocess_and_write_data5(seqs(bt),bulges1(bt),bulges2(bt),endbulges(bt), trn_filename5,
pos(bt));
    disp('written preprocessed training examples');

    dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename5 ' ' model_filename5]);
    dos(['d:/svm_light/svm_classify ' tst_filename5 ' ' model_filename5 ' ' out_filename5]);
    dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename3 ' ' model_filename3]);
    dos(['d:/svm_light/svm_classify ' tst_filename3 ' ' model_filename3 ' ' out_filename3]);

    load(out_filename3);
    load(out_filename5)
    out5m = out5mb;
    out3m = out3mb;

    %[pos3m, score3m] = svm_position(x3s,out3m,seqno3s, endbulges(bs), lenp(bs));
    %[pos5m, score5m] = svm_position(x5s,out5m,seqno5s, endbulges(bs), lenp(bs));
%collect global variables
    x3 = [x3; x3s];

```

```

out3 =[out3;out3m];
if m == 1
    seqno3 = seqno3s;
else
    mx3 = max(seqno3);
    seqno3 = [seqno3 ; mx3+seqno3s];
end
% pos3 = [pos3 pos3m];
% score3 = [score3 score3m];

x5 = [x5;x5s];;
out5 =[out5;out5m];
if m == 1
    seqno5 = seqno5s;
else
    mx5 = max(seqno5);
    seqno5 = [seqno5 ; mx3+seqno5s];
end
% pos5 = [pos5 pos5m];
% score5 = [score5 score5m];
m = m+1;
end
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
disp(' ');
disp('*****');
disp('5 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) ]);
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params3.dat');
disp(' ');
disp('*****');
disp('3 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) ]);
disp(['svm light params: ' svm_params]);% perform m fold cross validation on article + zucker results by splitting set
% modified file names for input/output so that can be run in parralel
mfold = 5;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
svm_params = input('enter svm parameters: ','s');
model_filename5 = 'd:/svm_light/model5m_b';
tst_filename5 = 'd:/rosetta/svm_light_utils1/svm_tst_5m_b.dat';
trn_filename5 = 'd:/rosetta/svm_light_utils1/svm_trn_5m_b.dat';
out_filename5 = 'd:/rosetta/svm_light_utils1/out5m_b.out';
x5 = zeros(0);
out5 =zeros(0);
seqno5 = zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
    % test set

```

```

[x5s, seqno5s] = preprocess_and_write_data5(seqs(bs),bulges1(bs), ...
    bulges2(bs),endbulges(bs), tst_filename5);
disp(['m = ' num2str(m)]);
disp('written preprocessed test examples');

bt = setdiff(bins_all , bs);

[x5t, seqno5t] = preprocess_and_write_data5(seqs(bt),bulges1(bt),...
    bulges2(bt),endbulges(bt), trn_filename5, pos(bt));
disp('written preprocessed training examples');

dos(['d:/svm_light/svm_learn ' svm_params ' ' trn_filename5 ' ' model_filename5]);
dos(['d:/svm_light/svm_classify ' tst_filename5 ' ' model_filename5 ' ' out_filename5]);

load out5m_b.out

%collect global variables
x5 = [x5;x5s];;
out5 =[out5;out5m_b];
if m == 1
    seqno5 = seqno5s;
else
    mx5 = max(seqno5);
    seqno5 = [seqno5 ; mx5+seqno5s];
end
m = m+1;
end
clear x5s x5t out5m_b seqno5s seqno5t bs bt
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
disp(' ');
disp('*****');
disp('5 prime end');
disp(['params      : ' num2str([Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength]) '']);
disp(['svm light params: ' svm_params]);
%mfold_cvk
mfold = 8;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
k = 4;
pos5 = zeros(0);
score5 =zeros(0);
m = 1;
while m <= mfold
    bs = [bins(m)+1 : bins(m+1)];% test set
    bt = setdiff(bins_all , bs);% train set

    disp(['m = ' num2str(m)]);

```



```

[pos5m,score5m] = edit_predictk(seqsd(bt), seqs(bs), endbulges(bs),k);

pos5 = [pos5,pos5m];
score5 =[score5,score5m];

m = m+1;
end
function [intseq, fault_seq] = nuc2int4_new(strseq);
%[intseq, fault_seq] = nuc2int4_new(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
intseq = zeros(size(strseq));
fault_seq = 0;
for i = 1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i) = 1;
        case 'C' , intseq(i) = 2;
        case 'T' , intseq(i) = 3;
        case 'G' , intseq(i) = 4;
        otherwise , intseq = []; fault_seq = 1; break;
    end
end
function run_edit_distance()
infile='c:\editdistance\draw_file.dat';
outfile='c:\editdistance\dicer_res.dat';
cd \\rosetta4\Development\gideon\edit_dist
seqsd = cell(0);
ii=0
fid=fopen('seqsd','r');
while ~feof(fid)
    ii=ii+1;
    seqsd{ii}=fgetl(fid);

end
fclose(fid);
fidin = fopen(infile,'r');
fidout = fopen(outfile,'w');
fidin
seqstot = 1000; %number of sequences to classify each loop
seq_id0 = 0;
while ~feof(fidin)
    disp('reading structure...');
    [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fidin, seqstot);
    [pos,score] = edit_predict(seqsd, seqs, endbulges)

%write to file
%seq_id0 is added so as to sequential order of sequence numbers
seq_id = seq_id + seq_id0;
res = [seq_id; pos; score];
fprintf(fidout, '%d %d %g ', res);
seq_id0 = max(seq_id);

```

```

end
fclose(fidin);
fclose(fidout);
quit
return;
function y = prctile(x,p);
%PRCTILE gives the percentiles of the sample in X.
% Y = PRCTILE(X,P) returns a value that is greater than P percent
% of the values in X. For example, if P = 50 Y is the median of X.
%
% P may be either a scalar or a vector. For scalar P, Y is a row
% vector containing Pth percentile of each column of X. For vector P,
% the ith row of Y is the P(i) percentile of each column of X.
% Copyright (c) 1993-98 by The MathWorks, Inc.
% $Revision: 2.6 $ $Date: 1997/11/29 01:46:27 $
[prows pcols] = size(p);
if prows ~= 1 & pcols ~= 1
    error('P must be a scalar or a vector.');
```

```

end
if any(p > 100) | any(p < 0)
    error('P must take values between 0 and 100');
```

```

end
xx = sort(x);
[m,n] = size(x);
if m==1 | n==1
    m = max(m,n);
    if m == 1,
        y = x*ones(length(p),1);
        return;
    end
    n = 1;
    q = 100*(0.5:m - 0.5)./m;
    xx = [min(x); xx(:); max(x)];
else
    q = 100*(0.5:m - 0.5)./m;
    xx = [min(x); xx; max(x)];
end
q = [0 q 100];
y = interp1(q,xx,p);
function seqtable = prepare_seqtable(seqno_list);
% seqtable = prepare_seqtable(seqno);
%seqtable contains for each seqno its starting location in example list
% and its end location
seqtable = zeros(max(seqno_list),2);
i = 1;
seqno = seqno_list(i);
while i <= length(seqno_list)
    seqtable(seqno,1) = i;
    while seqno_list(i) == seqno
        seqtable(seqno,2) = i;
```

```

    i = i+1;
    if i > length(seqno_list)
        break
    end
end
if i > length(seqno_list)
    break
end
seqno = seqno_list(i);
end
return

```

```

function [x12, seqno] = preprocess_and_write_data3(seqsp,bulges1,bulges2,endbulges, filename, pos)
%[x12, seqno] = preprocess_and_write_data3(seqsp,bulges1,bulges2,endbulges,filename, pos+lend-1);
%[x12, seqno] = preprocess_and_write_data3(seqsp,bulges1,bulges2,endbulges,filename); %testing mode
% notice that here pos is pos
%x12 are the first two elements of x (side , relative_loopdist)
%high level function for preparing data and writing for svm training
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params3.dat');
if nargin == 5
    mode = 'testing';
else
    mode = 'training';
end
x12 = zeros(0);
seqno = zeros(0);
fid = fopen(filename,'w');
for i = 1:length(seqsp)
    if strcmp(mode,'training')
        [xi, yi] = preprocess3(seqsp{i},bulges1{i},bulges2{i},endbulges{i},pos(i));
    elseif strcmp(mode,'testing')
        [xi, yi] = preprocess3(seqsp{i},bulges1{i},bulges2{i},endbulges{i},NaN);
    end
    write_examples(xi, yi, fid);
    x12 = [x12; xi(:,1:2)];
    seqno = [seqno; i*ones(size(xi,1),1)];

    if mod(i,100) == 0; i, end
end
fclose(fid);
return

function [x12, seqno] = preprocess_and_write_data3(seqsp,bulges1,bulges2,endbulges, filename, pos)
%[x12, seqno] = preprocess_and_write_data3(seqsp,bulges1,bulges2,endbulges,filename, pos+lend-1);
%[x12, seqno] = preprocess_and_write_data3(seqsp,bulges1,bulges2,endbulges,filename); %testing mode
% notice that here pos is pos
%x12 are the first two elements of x (side , relative_loopdist)

```

```

%high level function for preparing data and writing for svm training
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params3.dat');
if nargin == 5
    mode = 'testing';
else
    mode = 'training';
end
x12 = zeros(0);
seqno = zeros(0);
fid = fopen(filename,'a');
for i = 1:length(seqsp)
    if strcmp(mode,'training')
        [xi, yi] = preprocess3(seqsp{i},bulges1{i},bulges2{i},endbulges{i},pos(i));
    elseif strcmp(mode,'testing')
        [xi, yi] = preprocess3(seqsp{i},bulges1{i},bulges2{i},endbulges{i},NaN);
    end
    write_examples(xi, yi, fid);
    x12 = [x12; xi(:,1:2)];
    seqno = [seqno; i*ones(size(xi,1),1)];

    if mod(i,100) == 0; i, end
end
fclose(fid);
return
function [x12, seqno] = preprocess_and_write_data5(seqsp,bulges1,bulges2,endbulges, filename, pos)
%[x12, seqno] = preprocess_and_write_data5(seqsp,bulges1,bulges2,endbulges,filename, pos);
%[x12, seqno] = preprocess_and_write_data5(seqsp,bulges1,bulges2,endbulges,filename); %testing mode
%x12 are the first two elements of x (side , relative_loopdist)
%high level function for preparing data and writing for svm training
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
if nargin == 5
    mode = 'testing';
else
    mode = 'training';
end
%Maxsize is a simple upper bound for the number of possible positions
Maxsize = 0;
for i = 1:length(seqsp);
    Maxsize = Maxsize+length(seqsp{i});
end
x12 = zeros(Maxsize,2);
seqno = zeros(Maxsize,1);
xfrom = 1; % index where to write into xi and seqno
fid = fopen(filename,'w');
for i = 1:length(seqsp)

```

```

if strcmp(mode,'training')
    [xi, yi] = preprocess5(seqsp{i},bulges1{i},bulges2{i},endbulges{i},pos(i));
elseif strcmp(mode,'testing')
    [xi, yi] = preprocess5(seqsp{i},bulges1{i},bulges2{i},endbulges{i},NaN);
end

write_examples(xi, yi, fid);
xlength = size(xi,1);

x12(xfrom: xfrom + xlength-1,:) = xi(:,1:2);
seqno(xfrom: xfrom + xlength-1) = i*ones(xlength,1);
xfrom = xfrom + xlength ;

if mod(i,1000) == 0; disp(i); end
end
fclose(fid);
% remove the unneeded sapce in x12 and seqno
x12(xfrom:Maxsize,:) = [];
seqno(xfrom:Maxsize) = [];
return
function [x12, seqno] = preprocess_and_write_data5(seqsp,bulges1,bulges2,endbulges, filename, pos)
%[x12, seqno] = preprocess_and_write_data5(seqsp,bulges1,bulges2,endbulges,filename, pos);
%[x12, seqno] = preprocess_and_write_data5(seqsp,bulges1,bulges2,endbulges,filename); %testing mode
%x12 are the first two elements of x (side , relative_loopdist)
%high level function for preparing data and writing for svm training
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
if nargin == 5
    mode = 'testing';
else
    mode = 'training';
end
x12 = zeros(0);
seqno = zeros(0);
fid = fopen(filename,'a');
for i = 1:length(seqsp)
    if strcmp(mode,'training')
        [xi, yi] = preprocess5(seqsp{i},bulges1{i},bulges2{i},endbulges{i},pos(i));
    elseif strcmp(mode,'testing')
        [xi, yi] = preprocess5(seqsp{i},bulges1{i},bulges2{i},endbulges{i},NaN);
    end

    write_examples(xi, yi, fid);
    x12 = [x12; xi(:,1:2)];
    seqno = [seqno; i*ones(size(xi,1),1)];

    if mod(i,100) == 0; i, end
end
fclose(fid);

```

```

return
function [x,y,seqno] = preprocess_data3(seqsp,bulges1,bulges2,endbulges,pos)
%[x,y,seqno] = preprocess_data3(seqsp,bulges1,bulges2,endbulges,pos); % for training
%[x,y,seqno] = preprocess_data3(seqsp,bulges1,bulges2,endbulges); % for testing
%
% 3' side of MiR
%
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
[Nnucfrom, Nnucto, Nbfrom, Nbto, Mindlength] = read_params('params3.dat');
if nargin == 5
    mode = 'training';
else
    mode = 'testing';
end
x = zeros(0);
y = zeros(0);
seqno = zeros(0);
if strcmp(mode,'training')
    for i = 1:length(seqsp)
        [xi, yi] = preprocess3(seqsp{i},bulges1{i},bulges2{i},endbulges{i},pos(i));
        x = [x; xi];
        y = [y; yi];
        seqno = [seqno; i*ones(size(yi))];
        if mod(i,10) == 0; i, end
    end
else
    for i = 1:length(seqsp)
        [xi, yi] = preprocess3(seqsp{i},bulges1{i},bulges2{i},endbulges{i});
        x = [x; xi];
        y = [y; yi]; % this is just a list of zeros
        seqno = [seqno; i*ones(size(yi))];
        if mod(i,10) == 0; i, end
    end
end
returnfunction [x,y,seqno] = preprocess_data5(seqsp,bulges1,bulges2,endbulges,pos)
%[x,y,seqno] = preprocess_data5(seqsp,bulges1,bulges2,endbulges,pos); % for training
%[x,y,seqno] = preprocess_data5(seqsp,bulges1,bulges2,endbulges); % for testing
%high level function for preparing data for svm training
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
Nnucfrom = -2; % nucleotides region of interest
Nnucto = 7;
Nbfrom = -2; %bulges region of interest
Nbto = 6;
Min_dlength = 17; % min dicer length
if nargin == 5
    mode = 'training';
else
    mode = 'testing';
end

```

```

end
x = zeros(0);
y = zeros(0);
seqno = zeros(0);
if strcmp(mode,'training')
    for i = 1:length(seqsp)
        [xi, yi] = preprocess5(seqsp{i},bulges1{i},bulges2{i},endbulges{i},pos(i));
        x = [x; xi];
        y = [y; yi];
        seqno = [seqno; i*ones(size(yi))];
        if mod(i,10) == 0; i, end
    end
else
    for i = 1:length(seqsp)
        [xi, yi] = preprocess5(seqsp{i},bulges1{i},bulges2{i},endbulges{i});
        x = [x; xi];
        y = [y; yi]; % this is just a list of zeros
        seqno = [seqno; i*ones(size(yi))];
        if mod(i,10) == 0; i, end
    end
end
returnfunction x = preprocess_window(posj, seqwin,bulges1win,bulges2win, seq_size, eb_size, eb_begin, eb_end)
%preprocess_window : lower level function
% produces a feature vector from 3windows of the sequence
global Nnucfrom Nnucto Nbfrom Nbto mode
lenx = 2 + length(seqwin) *4 + 2*length(bulges1win);
x = zeros(0);
side = sign(posj-eb_begin);
x(1) = side; % -1 for upper, 1 for lower
loopdist = (1 + side)/2 * (posj - eb_end) + ... % lower part
(1 -side)/2* (eb_begin - posj); % upper part
% normalize x2 by palyndrom available length
x(2) = loopdist/(0.5* (seq_size - eb_size));
n_assigned = 2;
binseq = zeros(4, Nnucto+1-Nnucfrom);
binseq([0:size(binseq,2)-1]*4 + seqwin) = 1;
binseq = binseq(:)';
x(n_assigned+1: n_assigned +length(binseq)) = binseq;
n_assigned = n_assigned + length(binseq);
x(n_assigned+1: n_assigned +2*length(bulges1win)) = [bulges1win bulges2win];
returnfunction [xi, yi] = preprocess3(seqspi,bulges1i,bulges2i,endbulgesi,posi)
% low level function aimed at processing a sigle sequence
%in testing mode, yi are simply 0;
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
seq_size = length(seqspi); % size of palindrome = # nucleotides
l = find(endbulgesi);
eb_size = length(l); % size of endbulge = loop
eb_begin = l(1);
eb_end = l(eb_size);

```

```

xi = zeros(0);
yi = zeros(0);
% range include for upper and lower 5' positions
from = min(Nbfrom,Nnucfrom);
to = max(Nbto, Nnucto);
for side = -1:2:1
    if side == -1
        posrange = Min_dlength : eb_begin-1-to;
    else
        posrange = eb_end+Min_dlength : seq_size-to;
    end

    for j = 1:length(posrange)
        posj = posrange(j);

        nuc_win = posj+Nnucfrom:posj+Nnucto; %window of nucleotides (sequence)
        b_win = posj+Nbfrom:posj+Nbto; %window of bulges (1 sided & 2 sided)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
        if length(seqspi) < max(nuc_win)
            disp('bug1')
        end
        if length(bulges1i) < max(b_win)| length(bulges2i) < max(b_win)
            disp('bug2')
        end
    end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

    xij = preprocess_window(posj, seqspi(nuc_win), ...
        bulges1i(b_win),bulges2i(b_win), seq_size, eb_size, eb_begin, eb_end);
    xi = [xi; xij];
    if strcmp(mode,'training')
        yij = (posj == posi)*2-1; %+1 or -1
        yi = [yi ; yij];
    else
        yi = [yi ; 0];
    end
end % for j = 1:length(posrange)
end % if side ==

returnfunction [xi, yi] = preprocess5(seqspi,bulges1i,bulges2i,endbulgesi,posi)
% low level function aimed at processing a sigle sequence
%in testing mode, yi are simply 0;
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
%disp('preprocess5 modified. target id triangle like near 5 prime end');
seq_size = length(seqspi); % size of palindrome = # nucleotides
l = find(endbulgesi);
eb_size = length(l); % size of endbulge = loop
eb_begin = l(1);
eb_end = l(eb_size);

```



```

xi = zeros(0);
yi = zeros(0);
% range include for upper and lower 5' positions
from = min(Nbfrom,Nnucfrom);
to = max(Nbto, Nnucto);
for side = -1:2:1
    if side == -1
        posrange = 1+abs(from) :eb_begin-Min_dlength;
    else
        posrange = eb_end+1+abs(from) : seq_size+1-Min_dlength;
    end

    for j = 1:length(posrange)
        posj = posrange(j);

        nuc_win = posj+Nnucfrom:posj+Nnucto; %window of nucleotides (sequence)
        b_win = posj+Nbfrom:posj+Nbto; %window of bulges (1 sided & 2 sided)
        xij = preprocess_window(posj, seqspi(nuc_win), ...
            bulges1i(b_win),bulges2i(b_win), seq_size, eb_size, eb_begin, eb_end);
        xi = [xi; xij];

        if strcmp(mode,'training')
            yij = (posj == posi)*2-1; %+1 or -1
            % new version suitable for regression
            %yij = max(1-0.5*abs(posj-posi), -1); % giving 1 at max and -1 at distance 3 or more
            yi = [yi ; yij];
        else
            yi = [yi ; 0];
        end
    end % for j = 1:length(posrange)
end % if side ==

return[pos5,score5] = svm_position(x5,out5, seqno5, endbulges, lenp);
svkernel = input('enter kernel name: ','s');
targetdir = input('enter target directory name (e.g.) params-1-10-1-10: ','s');
targetfile = ['d:\rosetta\svm_light_utils\figures_174\' targetdir '\ svkernel];
figure(1); analyse_errors_thresh(pos5,score5,pos,endbulges); title(svkernel);
eval(['print -djpeg90 ' targetfile 'thresh']);
figure(2); analyse_errors_perc(pos5,score5,pos,endbulges); title(svkernel);
eval(['print -djpeg90 ' targetfile 'perc']);
in='c:\rosetta\data_baseline_15_5\draw_file2K.dat';
o = 'edist_res_file_hmdc257_2000pals.txt';
run_edit_distance_ranit(in,o);
in='c:\rosetta\data_baseline_15_5\200VirusesDraw.txt';
o = 'edist_res_file_hmdc257_virus.txt';
run_edit_distance_ranit(in,o);
in='c:\rosetta\data_baseline_15_5\badPalsGrade.txt';
o = 'edist_res_file_hmdc257_lowpal.txt';
run_edit_distance_ranit(in,o);
in='c:\rosetta\data_baseline_15_5\goodPalsGrade33.txt';
o = 'edist_res_file_hmdc257_highpal.txt';

```

```

run_edit_distance_ranit(in,o);function [Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params(paramsfile);
%[Nnucfrom, Nnucto, Nbfrom, Nbto, Mindlength] = read_params(paramsfile);
Nfields = 5;
fieldnames = cell(Nfields);
fieldnames(1:Nfields) = {'Nnucfrom'; 'Nnucto'; 'Nbfrom'; 'Nbto' ; 'Min_dlength'};
fid = fopen(paramsfile,'r');
while ~feof(fid)
    line = fgetl(fid);
    [field, rest] = strtok(line);

    if ~isempty(rest)
        value = num2str(strtok(rest));
    else
        error(['value of ' field ' not specified']);
    end

    % assign the value to the proper variable
    found = 0;
    for i = 1:Nfields
        if strcmp(field, fieldnames{i})
            eval(['field '=' num2str(value) ']);
            found = 1;
            break
        end
    end
    if found == 0
        error(['illegal field ' field ]);
    end
end
fclose(fid);
return

```

```

function [seqs,len] = read_seq(filename);
%[len,seqs] = read_seq(filename);
%reads dicer or pal sequences into cell array, in numeric format
fid = fopen(filename,'r');
if fid == -1
    error(['file ' filename ' could not be opened']);
end
id = 0;
seq_no = 0;
while ~feof(fid)
    line = fgetl(fid);
    line = deblank(line);
    [intseq, fault_seq] = nuc2int4_new(line);
    id = id + 1;
    if fault_seq == 0
        seq_no = seq_no + 1;
        seqs{seq_no} = intseq;
        len(seq_no) = length(intseq);
    end
end

```

```

else
    disp(['faulty seq on id ' num2str(id)])
end

if(mod(seq_no,1000) == 0 & seq_no ~= 0)
    disp(['seq_no ' num2str(seq_no)]);
end
end
fclose(fid);
return

function [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure(filename);
%[seqs,bulges1,bulges2,endbulges,seq_id] = read_structure(filename)
% read zucker structure
% seq is a cell array containing sequences
% bulge1 is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
% bulge2 is similarly for 2 sided bulge
% endbulge is a cell array with binary strings with 1 on the end bulge only
Mxplen = 250; % maximal length of palindrom
if nargin == 0
    filename = 'C:\rosetta_versions\ver9\data\zucker_draw_z.txt';
end
fid = fopen(filename,'r');
seq_no = 0;
seqs = cell(0);
bulges1= cell(0);
bulges2= cell(0);
endbulges = cell(0);
seq_id = zeros(0);
id = 0;
while ~feof(fid)
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    id = id +1;
    [seqi, bulge1i, bulge2i, endbulgei] = get_features(structure);
    [intseq, fault_seq] = nuc2int4_new(seqi);
    if fault_seq == 0
        seq_no = seq_no + 1;
        seqs{seq_no} = intseq;
        bulges1{seq_no} = bulge1i;
        bulges2{seq_no} = bulge2i;
        endbulges{seq_no} = endbulgei;
        seq_id(seq_no) = id;
    else
        disp(['faulty seq on id ' num2str(id)])
    end
    if(mod(seq_no,1000) == 0)

```

```

        seq_no
    end
end
fclose(fid);
return
function [seq, bulge1, bulge2, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
for col = 1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col = max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
    end
end

```

```

    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
    endbulge(count) = 0;
end
end
return

```

```

function [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fid,seqtot);
%[seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fid,seqtot)
% file id version: read 'seqtot' zucker draw palindromes from file handle 'fid'
%
% read zucker structure
% seq is a cell array containing sequences
% bulge1 is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
% bulge2 is similarly for 2 sided bulge
% endbulge is a cell array with binary strings with 1 on the end bulge only
Mxplen = 250; % maximal length of palindrom
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
[Nnucfrom, Nnucto, Nbfrom, Nbto, Min_dlength] = read_params('params5.dat');
seq_no = 0;
seqs = cell(0);
bulges1= cell(0);
bulges2= cell(0);
endbulges = cell(0);
seq_id = zeros(0);
id = 0;
while ~feof(fid) & seq_no < seqtot
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    id = id +1;
    [seqi, bulge1i, bulge2i, endbulgei] = get_features(structure);
    [intseq, fault_seq] = nuc2int4_new(seqi);
    fault_structure = check_structure(seqi, bulge1i, bulge2i, endbulgei);

    if fault_seq == 0 & fault_structure == 0
        seq_no = seq_no + 1;
        seqs{seq_no} = intseq;
        bulges1{seq_no} = bulge1i;
        bulges2{seq_no} = bulge2i;
        endbulges{seq_no} = endbulgei;
        seq_id(seq_no) = id;
    end
end

```

```

else
    disp(['faulty seq on id ' num2str(id)])
end
if(mod(seq_no,1000) == 0)
    seq_no
end
end
return
function [seq, bulge1, bulge2, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
for col = 1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
pos = length(bulge1);
if(pos < 1)
    return
end
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);

```

```

for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
return
function fault_structure = check_structure(seq_i, bulge1_i, bulge2_i, endbulge_i)
%test whether structure can be worked out by classifier, e.g.
% length of sequence is too short not enough space for Mir of length Mindlength
global Nnucfrom Nnucto Nbfrom Nbto mode
global Min_dlength
seq_size = length(seq_i);
lb = find(endbulge_i);
if(isempty(lb))
    fault_structure=1
    return
end
eb_size = length(lb);
eb_begin = lb(1);
eb_end = lb(eb_size);
% how many nucleotides/bulges are taken before 5' position
from = min(Nbfrom,Nnucfrom);
if (1+abs(from) > eb_begin-Min_dlength) & ...
    (eb_end+1+abs(from) > seq_size+1-Min_dlength)
    fault_structure = 1;
else
    fault_structure = 0;
end
return

function [seqs,bulges1,bulges2,endbulges,seq_id, conn] = read_structure_new(filename);
%[seqs,bulges1,bulges2,endbulges,seq_id,conn] = read_structure_new(filename)
% read zucker structure
% updated 22.1
% extractes also connection structure:
% conn(i) = index of nucleotide connected to nucleotide i (0 if unconnected);
% seq is a cell array containing sequences
% bulge1 is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
% bulge2 is similarly for 2 sided bulge

```

```

% endbulge is a cell array with binary strings with 1 on the end bulge only
Mxplen = 250; % maximal length of palindrom
if nargin == 0
    filename = 'C:\rosetta_versions\ver9\data\zucker_draw_z.txt';
end
fid = fopen(filename,'r');
seq_no = 0;
seqs = cell(0);
bulges1= cell(0);
bulges2= cell(0);
endbulges = cell(0);
seq_id = zeros(0);
conn = cell(0);
id = 0;
while ~feof(fid)
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    id = id + 1;
    [seqi, bulge1i, bulge2i, endbulgei, conni] = get_features(structure);
    [intseq, fault_seq] = nuc2int4_new(seqi);
    if fault_seq == 0
        seq_no = seq_no + 1;
        seqs{seq_no} = intseq;
        bulges1{seq_no} = bulge1i;
        bulges2{seq_no} = bulge2i;
        endbulges{seq_no} = endbulgei;
        seq_id(seq_no) = id;
        conn{seq_no} = conni;
    else
        disp(['faulty seq on id ' num2str(id)])
    end
    if(mod(seq_no,1000) == 0)
        seq_no
    end
end
return
function [seq, bulge1, bulge2, endbulge, conn] = get_features(structure)
% get sequence as well as bulge structure
% sequence index of nucleotide in structure
structure_seq_ind = zeros(size(structure));
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
[j,k] = find(isletter(structure(1:2,:)));
max_col = max(k);
count = 0;
for col =1: max_col

```



```

fl = find(isletter(structure(1:2,col)));
if ~isempty(fl)
    count = count + 1;
    seq(count) = structure(1:2,col);
    bulge = (fl == bulge_row);
    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
    structure_seq_ind(col, fl) = count;
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 4; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(structure(3:4,:)));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(structure(3:4,col)));
    if ~isempty(fl)
        fl = fl+2; % add 2 since fl = 1/2 on structure(3:4,:
        count = count + 1;
        seq(count) = structure(fl,col);
        bulge = (fl == bulge_row);
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
        structure_seq_ind(col, fl) = count;
    end
end
% produce connection structure
conn = zeros(size(seq));
[j,k] = find(structure_seq_ind(2:3,:) ~= 0);

```

```

j_opp = 5-j; %opposite to j. 3 <-> 2
% produce connection matrix in simple representation
for i = 1:length(j)
    conn(structure_seq_ind(j(i),k(i))) = structure_seq_ind(j_opp(i),k(i));
end
return
function [seqsd, seqs,bulges1,bulges2,endbulges,seq_id] = remove_duplicates(seqsd,
seqs,bulges1,bulges2,endbulges,seq_id);
%[seqsd, seqs,bulges1,bulges2,endbulges,seq_id] = remove_duplicates(seqsd,
seqs,bulges1,bulges2,endbulges,seq_id);
% locate only unique palindrome-dicer pairs
% dicers must be sorted lexicographically
if length(seqsd) ~= length(seqs)
    error('seqsd and seqs not compatible');
end
ldl = zeros(length(seqsd),1); %entries to be deleted
for i = 2:length(seqsd)
    if length(seqsd{i}) == length(seqsd{i-1}) & length(seqs{i}) == length(seqs{i-1})
        if all(seqsd{i} == seqsd{i-1}) & all(seqs{i} == seqs{i-1})
            ldl(i) = 1;
        end
    end
end
%delete duplicates
l = find(ldl);
seqsd(l) = [];
seqs(l) = [];
bulges1(l) = [];
bulges2(l) = [];
endbulges(l) = [];
seq_id(l) = [];
return

% perform a partitioned testing on large data
mfold = 3;
n_all = length(seqs);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
m = 1;
fname = 'res_poly3_33156.out';
fid = fopen(fname, 'a');
while m <= mfold
    bs = [bins(m)+1: bins(m+1)];
    % test set
    filename3 = ['svm3_33156m.dat'];
    filename5 = ['svm5_33156m.dat'];

    [x3s, seqno3s] = preprocess_and_write_data3(seqs(bs),bulges1(bs),bulges2(bs),endbulges(bs), filename3);
    [x5s, seqno5s] = preprocess_and_write_data5(seqs(bs),bulges1(bs),bulges2(bs),endbulges(bs), filename5);
    disp(['m = ' num2str(m)]);
end

```

```

disp('written preprocessed test examples');

disp('now run svm_classify. inputs are svm3_33156m.dat and svm5_33156m.dat');
disp('results should be in g:\research\rosetta\svm_light_utils1\svm_outputs\out3m.out, out5m.out');
disp('*****');

pause
cd svm_outputs

% test that both out files exist
files_ok = 0;
while files_ok == 0;
    files_ok = 1;
    fid5 = fopen('out5m.out','r');
    fid3 = fopen('out3m.out','r');

    if fid5 == -1
        files_ok = 0;
        disp('run svm_classify on 3 data. out3m.out not found. enter when ready');
        pause
    else
        fclose(fid5);
    end

    if fid3 == -1
        files_ok = 0;
        disp('run svm_classify on 3 data. out3m.out not found. enter when ready');
        pause
    else
        fclose(fid3);
    end
end

load out3m.out
load out5m.out
%delete files to insure that on next iteration, files are new
delete out3m.out
delete out5m.out

cd ..

[pos3m, score3m] = svm_position(x3s,out3m,seqno3s, endbulges(bs), lenp(bs));
[pos5m, score5m] = svm_position(x5s,out5m,seqno5s, endbulges(bs), lenp(bs));
[pos53m, score53m] = svm_position53(x5s,out5m,seqno5s, x3s,out3m,seqno3s, endbulges(bs), lenp(bs));

[yside, yprec2] = interpolate_probabilities(score53m, 'poly3');

res = [seq_id(bs); pos53m(:,1)'; pos53m(:,2)'; score53m'; yside'; yprec2'];
fprintf(fid, '%d %d %d %g %g %g\n', res);

```

```

    m = m+1;
end
fclose(fid);
function run_edit_distance()
%run_edit_distance(dicerfile, palfile, outfile)
fitfile = '\\rosetta4\\Development\\gideon\\edit_dist\\fit_21_025_1.txt'; %suitable for parameter alpha = 0.25
dicerfile='\\rosetta4\\Development\\gideon\\edit_dist\\seqsd'
palfile='c:\\editdistance\\draw_file.dat';
outfile='c:\\editdistance\\dicer_res.dat';
cd \\rosetta4\\Development\\gideon\\edit_dist
[seqsd,len] = read_seq(dicerfile);
%transform to string
length(seqsd)
for i = 1: length(seqsd)
    seqsd{i} = int2nuc(seqsd{i},'uppercase');
end
fidin = fopen(palfile,'r');
fidout = fopen(outfile,'a');
seqstot = 1000; %number of sequences to classify each loop
seq_id0 = 0;
while ~feof(fidin)
    disp('reading structure...');
    [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fidin, seqstot);

    %transform back to string
    for i = 1: length(seqs)
        seqs{i} = int2nuc(seqs{i},'uppercase');
    end

    [pos,score] = edit_predict(seqsd, seqs, endbulges)

    %write to file
    %seq_id0 is added so as to sequential order of sequence numbers
    seq_id = seq_id + seq_id0;

    % interpolate
    [yside, yprec2] = interpolate_prob_new(score, fitfile);
    res = [seq_id; pos; score; yprec2;yside];
    fprintf(fidout, '%d %d %g %g %g ', res);
    seq_id0 = max(seq_id);
end
fclose(fidin);
fclose(fidout);
quit
function run_edit_distance()
infile='c:\\editdistance\\draw_file.dat';
outfile='c:\\editdistance\\dicer_res.dat';
cd \\rosetta4\\Development\\gideon\\edit_dist
seqsd = cell(0);

```

```

ii=0
fid=fopen('seqsd','r');
while ~feof(fid)
    ii=ii+1;
    seqsd{ii}=fgetl(fid);

end
fclose(fid);
fidin = fopen(infile,'r');
fidout = fopen(outfile,'w');
fidin
seqstot = 1000; %number of sequences to classify each loop
seq_id0 = 0;
while ~feof(fidin)
    disp('reading structure...');
    [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fidin, seqstot);
    [pos,score] = edit_predict(seqsd, seqs, endbulges)

    %write to file
    %seq_id0 is added so as to sequential order of sequence numbers
    seq_id = seq_id + seq_id0;
    res = [seq_id; pos; score];
    fprintf(fidout, '%d %d %g ', res);
    seq_id0 = max(seq_id);
end
fclose(fidin);
fclose(fidout);
quit
return;

function run_edit_distance_ranit(palfile,outfile)
fitfile = 'fit_21_025_1.txt'; %suitable for parameter alpha = 0.25
dicerfile='seqsd_hmdc257';
[seqsd,len] = read_seq(dicerfile);
%transform to string
length(seqsd)
for i = 1: length(seqsd)
    seqsd{i} = int2nuc(seqsd{i},'uppercase');
end
fidin = fopen(palfile,'r');
fidout = fopen(outfile,'w');
seqstot = 1000; %number of sequences to classify each loop
seq_id0 = 0;
while ~feof(fidin)
    disp('reading structure...');
    [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fidin, seqstot);

    %transform back to string
    for i = 1: length(seqs)
        seqs{i} = int2nuc(seqs{i},'uppercase');
    end
end

```

```

[pos,score] = edit_predict(seqsd, seqs, endbulges)

%write to file
%seq_id0 is added so as to sequential order of sequence numbers
seq_id = seq_id + seq_id0;

% interpolate
[yside, yprec2] = interpolate_prob_new(score, fitfile);
res = [seq_id; pos; score; yprec2;yside];
fprintf(fidout, '%d %d %g %g %g\n', res);
seq_id0 = max(seq_id);
end
fclose(fidin);
fclose(fidout);
function [pos, score] = svm_position(x,svm_score,seqno, endbulges, lenp);
%[pos, score] = svm_position(x,svm_score, seqno, endbulges, lenp);
% postprocess svm outputs (for error analysis)
if size(x,1) ~= size(svm_score,1)
    error('x and svm_score not compatible');
end
if size(x,1) ~= size(seqno,1)
    error('x and seqno not compatible');
end
if max(seqno) ~= length(endbulges)
    error('seqno entries and endbulges size not compatible');
end
if length(lenp) ~= length(endbulges)
    error('lenp entries and endbulges size not compatible');
end
% use seqno to produce a list of boundaries between examples of different sequences
% this is important for efficiency (O(n) instead of O(n^2 log n))
ds = diff(seqno);
bnd = find(ds);
boundaries = [0 bnd' length(seqno)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
for s = 1:max(seqno)
    l = boundaries(s)+1 : boundaries(s+1);
    [maxs,m] = max(svm_score(l));
    score(s) = maxs;

    seq_size = lenp(s);
    lb = find(endbulges{s});
    eb_size = length(lb);
    eb_begin = lb(1);
    eb_end = lb(eb_size);

    side = x(l(m),1);
    loopdist = x(l(m),2) * (0.5* (seq_size - eb_size));
    pos(s) = (1+side)/2*(eb_end + loopdist) + (1-side)/2*(eb_begin - loopdist);
end

```

```

pos = round(pos);
returnfunction [pos, score] = svm_position_r(x,svm_score,seqno, endbulges, lenp);
%[pos, score] = svm_position_r(x,svm_score, seqno, endbulges, lenp);
% postprocess svm outputs (for error analysis)
% regression version
if size(x,1) ~= size(svm_score,1)
    error('x and svm_score not compatible');
end
if size(x,1) ~= size(seqno,1)
    error('x and seqno not compatible');
end
if max(seqno) ~= length(endbulges)
    error('seqno entries and endbulges size not compatible');
end
if length(lenp) ~= length(endbulges)
    error('lenp entries and endbulges size not compatible');
end
% use seqno to produce a list of boundaries between examples of different sequences
% this is important for efficiency (O(n) instead of O(n^2 log n))
ds = diff(seqno);
bnd = find(ds);
boundaries = [0 bnd' length(seqno)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
w = [-1.0 -0.5 0.0 0.5 1.0 0.5 0.0 -0.5 -1.0]; % window for convolution
nws = 0.5*(length(w)-1);
for s = 1:max(seqno)
    l = boundaries(s)+1 : boundaries(s+1);
    svm_scorel = svm_score(l);
    cnv = conv(w,svm_scorel);
    lcnv = length(cnv);
    % delete nws values on either side of cnv so that size equals that of scorel
    cnv([1:nws , lcnv-nws+1:lcnv]) = [];
    [maxs,m] = max(cnv);
    score(s) = maxs;

    seq_size = lenp(s);
    lb = find(endbulges{s});
    eb_size = length(lb);
    eb_begin = lb(1);
    eb_end = lb(eb_size);

    side = x(l(m),1);
    loopdist = x(l(m),2) * (0.5* (seq_size - eb_size));
    pos(s) = (1+side)/2*(eb_end + loopdist) + (1-side)/2*(eb_begin - loopdist);
end
pos = round(pos);
returnfunction [pos, score] = svm_position_soft(x,svm_score,seqno, endbulges, lenp);
%[pos, score] = svm_position_soft(x,svm_score, seqno, endbulges, lenp);
% postprocess svm outputs (for error analysis)
%
% takes the position closest to loop from positions which are at least

```

```

% best score - (1-Thresh)*abs(best score)
%
Thresh = 0.8;
if size(x,1) ~= size(svm_score,1)
    error('x and svm_score not compatible');
end
if size(x,1) ~= size(seqno,1)
    error('x and seqno not compatible');
end
if max(seqno) ~= length(endbulges)
    error('seqno entries and endbulges size not compatible');
end
if length(lenp) ~= length(endbulges)
    error('lenp entries and endbulges size not compatible');
end
% use seqno to produce a list of boundaries between examples of different sequences
% this is important for efficiency (O(n) instead of O(n^2 log n))
ds = diff(seqno);
bnd = find(ds);
boundaries = [0 bnd' length(seqno)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
for s = 1:max(seqno)
    seq_size = lenp(s);
    lb = find(endbulges{s});
    eb_size = length(lb);
    eb_begin = lb(1);
    eb_end = lb(eb_size);

    l = boundaries(s)+1 : boundaries(s+1);

    maxs = max(svm_score(l));
    score(s) = maxs;
    m = find(svm_score(l) >= maxs - (1-Thresh)*abs(maxs));
    loopdist = x(l(m),2) * (0.5* (seq_size - eb_size));
    minlpdst = min(loopdist);
    lminloopdist = find(loopdist == minlpdst);
    m = m(lminloopdist);
    if length(m) > 1
        mscore = svm_score(l(m));
        [mxs,i] = max(mscore);
        m = m(i);
    end

    side = x(l(m),1);
    loopdist = x(l(m),2) * (0.5* (seq_size - eb_size));
    pos(s) = (1+side)/2*(eb_end + loopdist) + (1-side)/2*(eb_begin - loopdist);
end
pos = round(pos);
returnfunction [pos, score] = svm_position53(x5,svm_score5, seqno5, x3, svm_score3, seqno3, endbulges, lenp);
%[pos, score] = svm_position53(x5,svm_score5, seqno5, x3, svm_score3, seqno3, endbulges, lenp);
% postprocess svm outputs (for error analysis)

```



```

global Maxpos
method = 'bestn';
param = 1;
Maxpos = 10; % maximal number of positions returned
alpha5 = 0.6; alpha3 = 0.40; alpha_dlen = 0.4; % relative weights of 5 and 3 predictions
disp(['alpha5 alpha3 alpha_dlen' num2str(alpha5) ' ' ...
     num2str(alpha3) ' ' num2str(alpha_dlen)]);
if size(x5,1) ~= size(svm_score5,1)
    error('x5 and svm_score5 not compatible');
end
if size(x3,1) ~= size(svm_score3,1)
    error('x3 and svm_score3 not compatible');
end
if size(x5,1) ~= size(seqno5,1)
    error('x5 and seqno5 not compatible');
end
if size(x3,1) ~= size(seqno3,1)
    error('x3 and seqno3 not compatible');
end
if max(seqno5) ~= max(seqno3)
    error('seqno5 and seqno3 not compatible');
end
if max(seqno5) ~= length(endbulges)
    error('seqno entries and endbulges size not compatible');
end
if length(lenp) ~= length(endbulges)
    error('lenp entries and endbulges size not compatible');
end
fid = fopen('d:\rosetta\svm_light_utils1\dicer_length.out','r');
dlen = str2num(fgetl(fid));
pdlen = str2num(fgetl(fid));
fclose(fid);
dlenmin = min(dlen);
dlenmax = max(dlen);
scdlen = log(pdlen); % scale to score - heuristic!!!
scdlen = scdlen + mean(scdlen);
nseq = max(seqno5);
% use seqno to produce a list of boundaries between examples of different sequences
% this is important for efficiency (O(n) instead of O(n^2 log n))
ds5 = diff(seqno5);
bnd5 = find(ds5);
boundaries5 = [0 bnd5' length(seqno5)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
ds3 = diff(seqno3);
bnd3 = find(ds3);
boundaries3 = [0 bnd3' length(seqno3)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
if strcmp(method, 'bestn')
    pos = zeros(nseq,2*param);
    score = zeros(nseq,param);
elseif strcmp(method, 'best plus other side')
    pos = zeros(nseq,2*2);

```

```

    score = zeros(nseq,2);
else
    error('not supported yest');
end
for s = 1:max(seqno5)
    l5 = boundaries5(s)+1 : boundaries5(s+1);
    l3 = boundaries3(s)+1 : boundaries3(s+1);

    score5 = svm_score5(l5);
    score3 = svm_score3(l3);

    seq_size = lenp(s);
    lb = find(endbulges{s});
    eb_size = length(lb);
    eb_begin = lb(1);
    eb_end = lb(eb_size);

    side5 = x5(l5,1);
    loopdist5 = x5(l5,2) * (0.5* (seq_size - eb_size));
    pos5 = (1+side5)/2.*(eb_end + loopdist5) + (1-side5)/2.*(eb_begin - loopdist5);
    pos5 = round(pos5);

    side3 = x3(l3,1);
    loopdist3 = x3(l3,2) * (0.5* (seq_size - eb_size));
    pos3 = (1+side3)/2.*(eb_end + loopdist3) + (1-side3)/2.*(eb_begin - loopdist3);
    pos3 = round(pos3);
    % initialize. pos53(:,1) contains 5' position , pos53(:,1) contains 3' position
    pos53 = zeros(length(l5)*size(pdlen,2),2);
    score53 = zeros(length(l5)*size(pdlen,2),1);
    count = 0;
    for i = 1:length(pos5);
        pos5i = pos5(i);
        J = find(pos3 >= pos5i + dlenmin - 1 & pos3 <= pos5i + dlenmax - 1 & side3 == side5(i));
        for j = 1:length(J);
            count = count+1;
            pos53(count,:) = [pos5i , pos3(J(j))];
            ind = pos3(J(j))-pos5i -dlenmin +2;
            if ind < 1 | ind > size(scdlen,2)
                disp('error')
            end

            score53(count) = alpha5*score5(i) + alpha3*score3(J(j)) + alpha_dlen*scdlen(ind);
            %score53(count) = alpha5*tanh(score5(i)) + alpha3*tanh(score3(J(j))) + alpha_dlen*scdlen(ind);
            %score53(count) = max(score5(i),score3(J(j))) + alpha_dlen*scdlen(ind);
        end
    end
    % now pick the desired positions for each sequence ,
    % e.g. 'best' , 'best plus other side', 'above thresh' 'percentile'.
    l = find(pos53(:,1) == 0);
    pos53(l,:) = [];

```

```

score53(l) = [];
if isempty(score53)
    error('empty score53');
end

[poss, scores] = choose_pos_score(pos53,score53, eb_begin, method, param);
pos(s,:) = poss;
score(s,:) = scores;
if mod(s,1000) == 0
    disp([num2str(s)])
end
end
return
function [pos, score] = choose_pos_score(pos53,score53, eb_begin, method, param)
% auxiliary function
if strcmp(method, 'bestn')
    nbest = param;
    [s,l] = sort(-score53);
    pos(1:nbest,:) = pos53(l(1:nbest),:);
    score(1:nbest) = score53(l(1:nbest));
    pos = pos';
    pos = pos(:);
    pos = pos';
    score = score';
elseif strcmp(method, 'best plus other side')
    pos = zeros(2,2);
    score = zeros(1,2);

    [mx,i] = max(score53);
    pos(1,:) = pos53(i,:);
    score(1) = score53(i);

    Os = find( (pos53(:,1)-eb_begin) * (pos(1,1) -eb_begin) < 0); %Other side
    if ~isempty(Os)
        [mx,i] = max(score53(Os));
        pos(2,:) = pos53(Os(i),:);
        score(2) = score53(Os(i));
    else
        % this may hapen when the sequence on other side was too short.
        pos(2,:) = NaN;
        score(2) = NaN;
    end
elseif strcmp(method, 'percentile')
    perc = params;
    if perc < 1
        perc = perc*100;
    end
    xp = prctile(score53, perc);
    l = find(score53 >= xp);
    [s,J] = sort(-score53(l));

```

```

J = l(J);
score = score53(l);
pos = pos53(l,:);
else
    error('method not implemented');
end
returnfunction [pos, score] = svm_position53h(x5,svm_score5, seqno5, x3, svm_score3, seqno3, endbulges, lenp);
%[pos, score] = svm_position53h(x5,svm_score5, seqno5, x3, svm_score3, seqno3, endbulges, lenp);
% postprocess svm outputs (for error analysis)
% hard limiter on results of classifier on 3'
global Maxpos
method = 'bestn';
param = 1;
Maxpos = 10; % maximal number of positions returned
alpha5 = 0.6; alpha3 = 0.40; alpha_dlen = 0.4; % relative weights of 5 and 3 predictions
disp(['alpha5 alpha3 alpha_dlen' num2str(alpha5) ' ' ...
    num2str(alpha3) ' ' num2str(alpha_dlen)]);
if size(x5,1) ~= size(svm_score5,1)
    error('x5 and svm_score5 not compatible');
end
if size(x3,1) ~= size(svm_score3,1)
    error('x3 and svm_score3 not compatible');
end
if size(x5,1) ~= size(seqno5,1)
    error('x5 and seqno5 not compatible');
end
if size(x3,1) ~= size(seqno3,1)
    error('x3 and seqno3 not compatible');
end
if max(seqno5) ~= max(seqno3)
    error('seqno5 and seqno3 not compatible');
end
if max(seqno5) ~= length(endbulges)
    error('seqno entries and endbulges size not compatible');
end
if length(lenp) ~= length(endbulges)
    error('lenp entries and endbulges size not compatible');
end
fid = fopen('d:\rosetta\svm_light_utils1\dicer_length.out','r');
dlen = str2num(fgetl(fid));
pdlen = str2num(fgetl(fid));
fclose(fid);
dlenmin = min(dlen);
dlenmax = max(dlen);
scdlen = log(pdlen); % scale to score - heuristic!!!
scdlen = scdlen + mean(scdlen);
nseq = max(seqno5);
% use seqno to produce a list of boundaries between examples of different sequences
% this is important for efficiency (O(n) instead of O(n^2 log n))
ds5 = diff(seqno5);

```

```

bnd5 = find(ds5);
boundaries5 = [0 bnd5' length(seqno5)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
ds3 = diff(seqno3);
bnd3 = find(ds3);
boundaries3 = [0 bnd3' length(seqno3)]; % examples of sequence i are between boundaries(i)+1 and boundaries(i+1)
if strcmp(method, 'bestn')
    pos = zeros(nseq,param);
    score = zeros(nseq,param);
elseif strcmp(method, 'best plus other side')
    pos = zeros(nseq,2);
    score = zeros(nseq,2);
else
    error('not supported yet');
end
for s = 1:max(seqno5)
    l5 = boundaries5(s)+1 : boundaries5(s+1);
    l3 = boundaries3(s)+1 : boundaries3(s+1);

    score5 = svm_score5(l5);
    score3 = svm_score3(l3);

    seq_size = lenp(s);
    lb = find(endbulges{s});
    eb_size = length(lb);
    eb_begin = lb(1);
    eb_end = lb(eb_size);

    side5 = x5(l5,1);
    loopdist5 = x5(l5,2) * (0.5* (seq_size - eb_size));
    pos5 = (1+side5)/2.*(eb_end + loopdist5) + (1-side5)/2.*(eb_begin - loopdist5);
    pos5 = round(pos5);

    if max(score3 < -0.1)
        [maxs,m] = max(svm_score5);
        score(s) = maxs;
        pos(s) = pos5(m);
    else
        side3 = x3(l3,1);
        loopdist3 = x3(l3,2) * (0.5* (seq_size - eb_size));
        pos3 = (1+side3)/2.*(eb_end + loopdist3) + (1-side3)/2.*(eb_begin - loopdist3);
        pos3 = round(pos3);
    % initialize. pos53(:,1) contains 5' position , pos53(:,1) contains 3' position
    pos53 = zeros(length(l5)*size(pdlen,2),1);
    score53 = zeros(length(l5)*size(pdlen,2),1);
    count = 0;
    for i = 1:length(pos5);
        pos5i = pos5(i);
        J = find(pos3 >= pos5i + dlenmin -1 & pos3 <= pos5i + dlenmax -1 & side3 == side5(i));
        for j = 1:length(J);
            count = count+1;

```

```

    pos53(count,:) = pos5i;
    ind = pos3(J(j))-pos5i -dlenmin +2;
    if ind < 1 | ind > size(scdlen,2)
        disp('error')
    end

    score53(count) = alpha5*score5(i) + alpha3*score3(J(j)) + alpha_dlen*scdlen(ind);
end
end
% now pick the desired positions for each sequence ,
% e.g. 'best' , 'best plus other side', 'above thresh' 'percentile'.
I = find(pos53(:,1) == 0);
pos53(I) = [];
score53(I) = [];
if isempty(score53)
    error('empty score53');
end

[poss, scores] = choose_pos_score(pos53,score53, eb_begin, method, param);
pos(s,:) = poss;
score(s,:) = scores;
if mod(s,1000) == 0
    disp([num2str(s)])
end
end
end
return
function [pos, score] = choose_pos_score(pos53,score53, eb_begin, method, param)
% auxiliary function
if strcmp(method, 'bestn')
    nbest = param;
    [s,I] = sort(-score53);
    pos(1:nbest) = pos53(I(1:nbest));
    score(1:nbest) = score53(I(1:nbest));
    pos = pos';
    score = score';
elseif strcmp(method, 'best plus other side')
    pos = zeros(1,2);
    score = zeros(1,2);

    [mx,i] = max(score53);
    pos(1) = pos53(i);
    score(1) = score53(i);

    Os = find( (pos53(:,1)-eb_begin) * (pos(1,1) -eb_begin) < 0); %Other side
    if ~isempty(Os)
        [mx,i] = max(score53(Os));
        pos(2) = pos53(Os(i));
        score(2) = score53(Os(i));
    else

```

```

        % this may hapen when the sequence on other side was too short.
        pos(2) = NaN;
        score(2) = NaN;
    end
elseif strcmp(method, 'percentile')
    perc = params;
    if perc < 1
        perc = perc*100;
    end
    xp = prctile(score53, perc);
    I = find(score53 >= xp);
    [s,J] = sort(-score53(I));
    J = I(J);
    score = score53(I);
    pos = pos53(I );
else
    error('method not implemented');
end
returnfunction svm_predict(infile,outfile);
%svm_predict(infile,outfile);
%perform svm position prediction
svm_light_folder = 'C:/svm/bin/';
model_filename5 = [svm_light_folder 'model5-2-6-2-6-21'];
tst_filename5 = 'C:/svm/Temp/svm_tst_5.dat';
svm_out_filename5 = 'C:/svm/Temp/out5.out';
fit_filename = 'C:/svm/Score/fit_p5-2-6-2-6-21.txt';
[seqs,bulges1,bulges2,endbulges,seq_id] = read_structure(infile);

[x5, seqno5] = preprocess_and_write_data5(seqs,bulges1, ...
    bulges2,endbulges, tst_filename5);
dos([svm_light_folder 'svm_classify ' tst_filename5 ' ' model_filename5 ' ' svm_out_filename5]);
% load and postprocess
curdir=pwd;
cd 'c:/svm/temp'
load out5.out;
cd(curdir);
lenp = length_seq(seqs);
[pos5, score5] = svm_position(x5,out5, seqno5, endbulges, lenp);
% infer probabilities
[yside, yprec2] = interpolate_prob_new(score5, fit_filename);
%write to file
res = [seq_id; pos5; score5; yprec2; yside];
fid = fopen(outfile,'w');
fprintf(fid, '%d %d %g %g %g\n', res);
fclose(fid);
function svm_predict();
%svm_predict_b(infile,outfile);
%perform svm position prediction
% version for large input files
% reads seqtot sequences at a time and classifies them

```

```

infile='c:\svm\in\draw_file.dat';
outfile='c:\svm\out\dicer_res.dat';
cd \\rosetta4\Development\gideon\svm\util
svm_light_folder = 'C:/svm/bin/';
model_filename5 = [svm_light_folder 'model5-2-6-2-6-21'];
tst_filename5 = 'C:/svm/Temp/svm_tst_5.dat';
svm_out_filename5 = 'C:/svm/Temp/out5.out';
fit_filename = 'C:/svm/Score/fit_p5-2-6-2-6-21.txt';
fidin = fopen(infile,'r');
fidout = fopen(outfile,'w');
seqstot = 1000; %number of sequences to classify each loop
seq_id0 = 0;
while ~feof(fidin)
    disp('reading structure...');
    [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fidin, seqstot);
    lenp = length_seq(seqs);

    disp('preprocessing and writing...');
    [x5, seqno5] = preprocess_and_write_data5(seqs,bulges1, ...
        bulges2,endbulges, tst_filename5);
    cd c:\
    dos([svm_light_folder 'svm_classify ' tst_filename5 ' ' model_filename5 ' ' svm_out_filename5]);
    cd \\rosetta4\Development\gideon\svm\util
% load and postprocess
fidsvm = fopen(svm_out_filename5,'r');
out5 = fscanf(fidsvm, '%g');
fclose(fidsvm);

    disp('postprocessing...');
    [pos5, score5] = svm_position(x5,out5, seqno5, endbulges, lenp);
% infer probabilities
    [yside, yprec2] = interpolate_prob_new(score5, fit_filename);
%write to file
%seq_id0 is added so as to sequential order of sequence numbers
    seq_id = seq_id + seq_id0;
    res = [seq_id; pos5; score5; yprec2; yside];
    fprintf(fidout, '%d %d %g %g %g ', res);
    seq_id0 = max(seq_id);
end
fclose(fidin);
fclose(fidout);
quit
function svm_predict_b(infile,outfile);
%svm_predict_b(infile,outfile);
%perform svm position prediction
% version for large input files
% reads seqtot sequences at a time and classifies them
svm_light_folder = 'C:/svm/bin/';
model_filename5 = [svm_light_folder 'model5-2-6-2-6-21'];
tst_filename5 = 'C:/svm/Temp/svm_tst_5.dat';

```



```

svm_out_filename5 = 'C:/svm/Temp/out5.out';
fit_filename = 'C:/svm/Score/fit_p5-2-6-2-6-21.txt';
fidin = fopen(infile,'r');
fidout = fopen(outfile,'w');
seqstot = 1000; %number of sequences to classify each loop
seq_id0 = 0;
while ~feof(fidin)
    disp('reading structure...');
    [seqs,bulges1,bulges2,endbulges,seq_id] = read_structure_fid(fidin, seqstot);
    lenp = length_seq(seqs);

    disp('preprocessing and writing...');
    [x5, seqno5] = preprocess_and_write_data5(seqs,bulges1, ...
        bulges2,endbulges, tst_filename5);
    dos([svm_light_folder 'svm_classify ' tst_filename5 ' ' model_filename5 ' ' svm_out_filename5]);
% load and postprocess
    fidsvm = fopen(svm_out_filename5,'r');
    out5 = fscanf(fidsvm, '%g');
    fclose(fidsvm);

    disp('postprocessing...');
    [pos5, score5] = svm_position(x5,out5, seqno5, endbulges, lenp);
% infer probabilities
    [yside, yprec2] = interpolate_prob_new(score5, fit_filename);
%write to file
%seq_id0 is added so as to sequential order of sequence numbers
    seq_id = seq_id + seq_id0;
    res = [seq_id; pos5; score5; yprec2; yside];
    fprintf(fidout, '%d %d %g %g %g\n', res);
    seq_id0 = max(seq_id);
end
fclose(fidin);
fclose(fidout);
function unique_seqs(seqs,seqsd,bulges1, bulges2, endbulges, lenp, lend, pos, seq_id)
[y,l] = sort(lenp);
bulges1 = bulges1(l);
bulges2 = bulges2(l);
endbulges = endbulges(l);
lend = lend(l);
lenp = lenp(l);
pos = pos(l);
seq_id = seq_id(l);
seqs = seqs(l);
seqsd = seqsd(l);

count = 1;
lc(count) = 1;
for i = 2:length(seqs)
    if lenp(i) == lenp(i-1)
        if any(seqs{i} ~= seqs{i-1})

```

```

        count = count+1;
        lc(count) = i;
    end
else
    count = count+1;
    lc(count) = i;
end
end

keyboard

function write_examples(xi,yi, fid);
% %low level function
% write examples in format compatible with svm light
% xi,yi are the example vector + targets
% in testing mode the yi's are set to 0
for j = 1:size(xi,1)
    fprintf(fid,'%d',yi(j));
    l = find(xi(j,:));
    xprint = [l;xi(j,l)];
    fprintf(fid,' %d:%g',xprint);
    fprintf(fid,'\n');
endfunction write_examples_simple(xi,yi, fid);
% %low level function
% write examples in format compatible with svm light
% xi,yi are the example vector + targets
% in testing mode the yi's are set to 0
for j = 1:size(xi,1)
    fprintf(fid,'%d',yi(j));
    fprintf(fid,' %g',xi);
    fprintf(fid,'\n');
end
kkk = 1:6000;
[x12_5, seqno_5] =
preprocess_and_write_data5(seqs(kk),bulges1(kk),bulges2(kk),endbulges(kk),'g:\research\rosetta\svm_light_utils1\sv
m_preprocessed\svm5_kk1.dat');
[x12_3, seqno_3] =
preprocess_and_write_data5(seqs(kk),bulges1(kk),bulges2(kk),endbulges(kk),'g:\research\rosetta\svm_light_utils1\sv
m_preprocessed\svm3_kk1.dat');
% use svm light to classify both each ewth its own model
load output5_kk1.out
load output3_kk1.out
[pos53kk, score53kk] = svm_position53(x12_5,output5_kk1, seqno_5, x12_3, output3_kk1, seqno_3, endbulges(kk),
lenp(kk));
%write final results to file
res = [seq_id(kk); pos53kk(:,1)'; pos53kk(:,2)'; score53kk'];
fid = fopen('res53_33156.out','a');
fprintf(fid, '%d %d %d %g\n', res);
fclose(fid);

```

```

function [first_pos,first_score] = firstk_determine(seqsd,seqs, pos1, pos2,ktup,k,range);
%[first_pos,first_score] = firstk_determine(seqsd,seqs, pos1, pos2,ktup,k,range);
%for each%for each palindrome with two mir predictions - which is better
%search on -2+2 positions on each side for the best firstk score
if nargin ==4
    model.ktup = 8;
    model.k = 1;
    model.range = -2:2;
else
    model.ktup = ktup;
    model.k = k;
    model.range = range;
end
model.beta = 2;
model.use_min = 0;
first_pos = zeros(size(seqs));
first_score = zeros(size(seqs));
for i = 1:length(seqs)
    if mod(i,100) == 0, fprintf('..%d',i);end
    [first_pos(i), first_score(i)] = firstk_determine1(seqsd,seqs{i}, pos1(i), pos2(i), model);
end
fprintf('\n');
return
function [first_posi, first_scorei] = firstk_determine1(seqsd,seqsi, pos1i, pos2i,model);
k = model.k;
ktup = model.ktup;
beta = model.beta;
range = model.range;
%around pos1
for i = 1:length(range)
    posi = pos1i+range(i);
    if posi >0 & posi +ktup <= length(seqsi)
        p = seqsi(posi:posi+ktup-1);
        for j = 1:length(seqsd)
            d(j) = editD(p,seqsd{j})(1:ktup));
        end
        min_d1(i) = min(d);
        % take also the mean of highest percentile
        [ds,l] = sort(d);
        mean_d1(i) = mean(ds(1:k));
    else
        mean_d1(i) = nan;
    end
end
end
max1 = 1-min(mean_d1)/ktup;
%around pos2
for i = 1:length(range)
    posi = pos2i+range(i);
    if posi >0 & posi +ktup <= length(seqsi)
        p = seqsi(posi:posi+ktup-1);

```

```

for j = 1:length(seqsd)
    d(j) = editD(p,seqsd{j})(1:ktup));
end
min_d2(i) = min(d);
% take also the mean of highest percentile
[ds,l] = sort(d);
    mean_d2(i) = mean(ds(1:k));
else
    mean_d2(i) = nan;
end
end
max2 = 1-min(mean_d2)/ktup;
if max1 > max2
    %first_posi = pos1i;
    first_posi = 1;
    first_scorei = max1;
elseif max2 > max1
    %first_posi = pos2i;
    first_posi = 2;
    first_scorei = max2;
else
    if model.use_min
        if min(min_d1) == min(min_d2)
            first_posi = nan;
            first_scorei = nan;
        elseif min(min_d1) < min(min_d2)
            first_posi = 1;
            first_scorei = 0;
        else
            first_posi = 2;
            first_scorei = 0;
        end
    else
        first_posi = nan;
        first_scorei = nan;
    end %if model.use_min
end
return
load vars_hmdc440
seqs = palseq;
seqsd = mirseq;
pos = mirpos;
lend = mirlen;
clear palseq mirseq mirpos mirlen curdir datadir
function [id, palgrade5, pal_seq, pos1, pos2, score] = read_table_res(filename)
%[id, palgrade5, pal_seq, pos1, pos2, score] = read_table_res(filename)
fid = fopen(filename,'r');
k = 1;
while ~feof(fid);
    if (mod(k,100) == 0) fprintf('.'); end

```

```

line = fgetl(fid);
if line(1) ~= '%'
    [t,r] = strtok(line);
    id(k) = str2num(t);
    [t,r] = strtok(r);
    palgrade5(k) = str2num(t);
    [t,r] = strtok(r);
    pal_seq{k} = t;
    [t,r] = strtok(r);
    pos1(k) = str2num(t);
    [t,r] = strtok(r);
    pos2(k) = str2num(t);
    [t,r] = strtok(r);
    score(k) = str2num(t);
    k = k+1;
end
end
fclose(fid);
return
function run_firstk_side_determine(filein, fileout)
%run_firstk_side_determine(filein, fileout)
%determine the better side of palgrade predictions, based of firstk
[id, palgrade5, pal_seq, pos1, pos2, score] = read_table_res(filein);
disp(['read ' num2str(length(id)) ' records']);
load_all;
seqsd_all = transform_format(seqsd);
%remove records with nan positions
l = find(isnan(pos1) | isnan(pos2));
id(l) = [];
palgrade5(l) = [];
pal_seq(l) = [];
pos1(l) = [];
pos2(l) = [];
score(l) = [];
disp([num2str(length(id)) ' non null records passed to firstk_determine']);
fid = fopen(fileout,'w');
[first_pos,first_score] = firstk_determine(seqsd_all,pal_seq, pos1, pos2,10, 3, -1:1);
res = [id; first_pos; first_score];
fprintf(fid, '%d %d %5.3f\n',res);
fclose(fid);
return

```

```

function bs_scoring_all_zukers_v5(infilename,outfilename)
% function bs_scoring_all_zukers_v5(infilename,outfilename)
% for each binding site, gives the score of all of its zucker versions, each
% score is between 0 and 1, where 1 is highest score.
% writes to the file outfilename in the format: bs_id zucker_version score bs_id...
% bs_id is as it appears in the input file (named infilename)
% see the paramfile and README for explanations on parameters
paramfilename = 'params5';
bs_tot = 1000;
eval(paramfilename);
fidout = fopen(outfilename,'w');
fidin = fopen(infilename,'r');
fprintf(fidout,'%%each line contains the following info:\r\n');
fprintf(fidout,'%%bs_id zucker_version score ratio_paired num_mir_bulges num_target_bulges sum_mir_tail_lens
bulge_kernel_mir num_gts\r\n');
while ~feof(fidin)
    a = read_brzucker(fidin,bs_tot);
    for i = 1:length(a)
        this_bs = a(i);
        for j=1:this_bs.numzukers
            z = this_bs.zukers(j);
            [s,f,ratio_paired,bulge_K,num_gts] = get_zucker_score_and_features(z,this_bs,params);
            if(f.has_draw == 0) % no draw available
                res = [nan nan nan nan nan nan];
            else
                res = [ratio_paired, f.num_mir_bulges, f.num_target_bulges,...
                    (f.mir_tail5_len+f.mir_tail3_len), bulge_K, num_gts];
            end
            fprintf(fidout,'%d %d %g %g %d %d %d %g %d\r\n',this_bs.bs_id,z.version,s,res);
        end
    end
end
fclose(fidin);
fclose(fidout);
function f_struct = features_from_zucker(zucker)
% function f_struct = features_from_zucker(zucker)
% zucker(i).draw_line1 is the string of the first of the 4 lines in the draw
% same for line2 thru line4. If no draw exists (rnastructure failed to draw)
% all lines are an 'X', and f.has_draw = 0. If there is a draw
% f.has_draw = 1, and f includes all the features extracted from the draw.
% f_struct(i) is a collection of fields describing this zucker.
% if there is only one zucker, f_struct is a single struct.
single_flag = 0;
if(length(zucker)==1)
    single_flag = 1;
    tt(1) = zucker;
    zucker = tt;
end
for i=1:length(zucker)
    z = zucker(i);

```

```

% -----
% correct lengths of strings to all same length
line1 = z.draw_line1;
line2 = z.draw_line2;
line3 = z.draw_line3;
line4 = z.draw_line4;
if(strcmp(upper(line1(1)), 'X'))
    f.has_draw = 0;
else
    f.has_draw = 1;
    f.energy = z.energy;
    tt = max([find(isletter(line1)), find(isletter(line2)), ...
        find(isletter(line3)), find(isletter(line4))]);
    line1 = [line1(1:min(tt, length(line1)))];
    for k=1:tt-length(line1); line1=[line1, ' ']; end
    line2 = [line2(1:min(tt, length(line2)))];
    for k=1:tt-length(line2); line2=[line2, ' ']; end
    line3 = [line3(1:min(tt, length(line3)))];
    for k=1:tt-length(line3); line3=[line3, ' ']; end
    line4 = [line4(1:min(tt, length(line4)))];
    for k=1:tt-length(line4); line4=[line4, ' ']; end
% -----
% find bulges and windows by order. bulge, win, bulge win etc
paired_wins_lens = [];
mir_bulge_vec = []; % of length as mir. 1 if on bulge, 0 else.
target_bulge_vec = []; % same for target.
if(isletter(line2(1)))
    in_bulge = 0;
    mir_bulges_lens = 0;
    target_bulges_lens = 0;
    this_win_len = 1;
else
    in_bulge = 1;
    if(isletter(line1(1)))
        this_mir_bulge = 1;
    else
        this_mir_bulge = 0;
    end
    if(isletter(line4(1)))
        this_target_bulge = 1;
    else
        this_target_bulge = 0;
    end
    mir_bulges_lens = [];
    target_bulges_lens = [];
end
for k=2:length(line1)
    if(isletter(line2(k)))
        if(in_bulge)
            in_bulge = 0;

```

```

        mir_bulges_lens = [mir_bulges_lens,this_mir_bulge];
        target_bulges_lens = [target_bulges_lens,this_target_bulge];
        this_win_len = 1;
    else
        this_win_len = this_win_len + 1;
    end
else
    if(in_bulge)
        if(isletter(line1(k)))
            this_mir_bulge = this_mir_bulge + 1;
        end
        if(isletter(line4(k)))
            this_target_bulge = this_target_bulge + 1;
        end
    else
        in_bulge = 1;
        paired_wins_lens = [paired_wins_lens,this_win_len];
        if(isletter(line1(k)))
            this_mir_bulge = 1;
        else
            this_mir_bulge = 0;
        end
        if(isletter(line4(k)))
            this_target_bulge = 1;
        else
            this_target_bulge = 0;
        end
    end
end
end
if(isletter(line2(end))) % finished in paired win
    mir_bulges_lens = [mir_bulges_lens,0];
    target_bulges_lens = [target_bulges_lens,0];
    paired_wins_lens = [paired_wins_lens,this_win_len];
else
    mir_bulges_lens = [mir_bulges_lens,this_mir_bulge];
    target_bulges_lens = [target_bulges_lens,this_target_bulge];
end
% get mir and target bulge vecs
mir_bulge_nonsym_vec = [];
mir_bulge_sym_vec = [];
target_bulge_nonsym_vec = [];
target_bulge_sym_vec = [];
L = length(mir_bulges_lens);
for k = 1:L
    ml = mir_bulges_lens(k);
    tl = target_bulges_lens(k);
    if(ml>0 & tl>0) % symmetric bulge
        mir_bulge_nonsym_vec = [mir_bulge_nonsym_vec,zeros(1,ml)];
        mir_bulge_sym_vec = [mir_bulge_sym_vec,ones(1,ml)];
    end
end

```



```

        target_bulge_nonsym_vec = [target_bulge_nonsym_vec,zeros(1,tl)];
        target_bulge_sym_vec = [target_bulge_sym_vec,ones(1,tl)];
elseif(ml>0 & tl==0)
    mir_bulge_nonsym_vec = [mir_bulge_nonsym_vec,ones(1,ml)];
    mir_bulge_sym_vec = [mir_bulge_sym_vec,zeros(1,ml)];
elseif(ml==0 & tl>0)
    target_bulge_nonsym_vec = [target_bulge_nonsym_vec,ones(1,tl)];
    target_bulge_sym_vec = [target_bulge_sym_vec,zeros(1,tl)];
else
end
if(k<L) % there is window after
    wl = paired_wins_lens(k);
    mir_bulge_nonsym_vec = [mir_bulge_nonsym_vec,zeros(1,wl)];
    mir_bulge_sym_vec = [mir_bulge_sym_vec,zeros(1,wl)];
    target_bulge_nonsym_vec = [target_bulge_nonsym_vec,zeros(1,wl)];
    target_bulge_sym_vec = [target_bulge_sym_vec,zeros(1,wl)];
end
end
% -----
% update related features in f.
f.paired_wins_lens_direction_5to3_onmir = paired_wins_lens;
f.num_paired_wins = sum(paired_wins_lens>0);
f.mir_bulges_lens_5to3 = mir_bulges_lens;
f.num_mir_bulges = sum(mir_bulges_lens>0);
f.target_bulges_lens_3to5 = target_bulges_lens;
f.num_target_bulges = sum(target_bulges_lens>0);
f.unified_bulges_lens = mir_bulges_lens + target_bulges_lens;
f.mir_tail5_len = mir_bulges_lens(1);
f.mir_tail3_len = mir_bulges_lens(end);
f.target_tail5_len = target_bulges_lens(end);
f.target_tail3_len = target_bulges_lens(1);
f.total_nucs = sum(2*paired_wins_lens) + ...
    sum(mir_bulges_lens) + sum(target_bulges_lens);
f.num_nucs_paired = sum(2*paired_wins_lens);
f.mir_nonsym_bulge_vec_5to3 = mir_bulge_nonsym_vec;
f.mir_sym_bulge_vec_5to3 = mir_bulge_sym_vec;
f.mir_bulge_vec_5to3 = mir_bulge_nonsym_vec + mir_bulge_sym_vec;
f.target_nonsym_bulge_vec_3to5 = target_bulge_nonsym_vec;
f.target_sym_bulge_vec_3to5 = target_bulge_sym_vec;
f.target_bulge_vec_5to3 = target_bulge_nonsym_vec + target_bulge_sym_vec;
% -----
end % if strcmp
f_struct(i) = f;
end % end loop on length(zuker)
if(single_flag)
    tt = f_struct(1);
    f_struct = tt;
end
function [score,f,ratio_paired,bulge_K,num_gts] = get_zuker_score_and_features(z,bs,params)
f = features_from_zuker(z); % f is a struct holding many features

```

```

if(f.has_draw == 0) % no draw available - give a score of 0!
    score = nan;
    ratio_paired = nan;
    bulge_K = nan;
    num_gts = nan;
    return;
end
ratio_paired = f.num_nucs_paired/f.total_nucs;
% normalize weights to sum of 1:
sum_ws = params.w_energy + params.w_ratio_paired + params.w_num_mir_bulges + ...
    params.w_num_target_bulges + params.w_mir_tail_lens + params.w_target_tail_lens + ...
    params.w_mir_bulge_kernel + params.w_gt_pairs;
w_energy = params.w_energy/sum_ws;
w_ratio_paired = params.w_ratio_paired/sum_ws;
w_num_mir_bulges = params.w_num_mir_bulges/sum_ws;
w_num_target_bulges = params.w_num_target_bulges/sum_ws;
w_mir_tail_lens = params.w_mir_tail_lens/sum_ws;
w_target_tail_lens = params.w_target_tail_lens/sum_ws;
w_mir_bulge_kernel = params.w_mir_bulge_kernel/sum_ws;
w_gt_pairs = params.w_gt_pairs/sum_ws;
[score_bk,bulge_K] = score_bulge_kernel(f.mir_bulge_vec_5to3,params.mir_bulge_pos_prices);
[score_gt,num_gts] = score_gt_pairs(z,params);
score = w_energy * min_max_score(params.min_energy,params.max_energy,-1,z.energy) + ...
    w_ratio_paired * ratio_paired + ...
    w_num_mir_bulges * min_max_score(params.min_num_mir_bulges,...
    params.max_num_mir_bulges,-1,f.num_mir_bulges) + ...
    w_num_target_bulges * min_max_score(params.min_num_target_bulges,...
    params.max_num_target_bulges,-1,f.num_target_bulges) + ...
    w_mir_tail_lens * min_max_score(params.min_mir_tail_lens,...
    params.max_mir_tail_lens,-1,(f.mir_tail5_len+f.mir_tail3_len)) + ...
    w_target_tail_lens * min_max_score(params.min_target_tail_lens,...
    params.max_target_tail_lens,-1,(f.target_tail5_len+f.target_tail3_len)) + ...
    w_mir_bulge_kernel * score_bk + w_gt_pairs * score_gt;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function score = min_max_score(min_v,max_v,dir_flag,value)
if(dir_flag == 1) % the higher the better
    score = (value - min_v)/(max_v - min_v);
elseif(dir_flag == -1) % the lower the better
    score = 1 - ((value - min_v)/(max_v - min_v));
else
    error('min_max_score: dir_flag must be 1 or -1. aborting');
end
if(score<0)
    score = 0;
    warning('min_max_score: encountered value outside range getting neg score. truncating score to 0');
end
if(score>1)
    score = 1;
    warning('min_max_score: encountered value outside range getting score higher than 1. truncating score to 1');

```

```

end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%
function [score,bulge_K] = score_bulge_kernel(bulge_vec,K)
l_vec = length(bulge_vec);
l_K = length(K);
r = floor(l_vec/l_K);
kernel = [];
for i = 1:l_K
    kernel = [kernel,K(i)*ones(1,r)];
end
kernel = [kernel,K(end)*ones(1,l_vec-r*l_K)];
kernel = kernel/sum(kernel);
bulge_K = sum(bulge_vec .* kernel); % weighted sum of bulges by position on vec
score = min_max_score(0,1,-1,bulge_K);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%
function [score,num_gts] = score_gt_pairs(z,params)
num_gts = 0;
for i=1:length(z.draw_line2)
    t1 = z.draw_line2(i);
    t2 = z.draw_line3(i);
    if((strcmp('G',t1) & strcmp('T',t2)) | (strcmp('T',t1) & strcmp('G',t2)))
        num_gts = num_gts + 1;
    end
end
end
score = min_max_score(params.min_num_gts,params.max_num_gts,-1,num_gts);params.choose_zuker_by = 'max';
% relevant only for bs_scoring_single_zuker
% range of energies. If the minimum is -30 and the max is 0 then the energy score of a
% zuker having energy -10 is 1/3. -30 will get a score of 1 etc. The score will be
% weighed also by w_energy.
params.max_energy = 0;
params.min_energy = -30;
% as above but for number of bulges
params.min_num_mir_bulges = 0;
params.max_num_mir_bulges = 6;
params.min_num_target_bulges = 0;
params.max_num_target_bulges = 6;
% again....
params.min_mir_tail_lens = 0;
params.max_mir_tail_lens = 15;
params.min_target_tail_lens = 0;
params.max_target_tail_lens = 15; % by default not using it anyways
% again...
params.min_num_gts = 0;
params.max_num_gts = 6;
% gives the pricing on bulges depending on position on mir
% if the vector is [1,0,1] then bulged nucs in the first and third third of the mir
% are penalized, while those in the middle third are not at all (basically
% a weighted sum).

```

```

% do not worry about normalization of this:
params.mir_bulge_pos_prices = [1,0,1];
% below the weights of each feature in the total score. The score of
% a zucker version is the sum of each of the individual scores times its
% weight. bs_scoring normalizes the sum of these to 1 (so here take care only of ratios)
params.w_energy = 1;
params.w_ratio_paired = 4;
params.w_num_mir_bulges = 0.5;
params.w_num_target_bulges = 0.5;
params.w_mir_tail_lens = 2;
params.w_target_tail_lens = 0; % should be 0 unless you have a very good reason to change
params.w_gt_pairs = 1;
params.w_mir_bulge_kernel = 1;
function brzucker_out_data = read_brzucker(fid,bs_tot)
% function brzucker_out_data = read_brzucker(fid,bs_tot)
% reads bs_tot binding sites at a time
% format of file:
% for each candidate binding site:
% > ofir's internal bs_id
% mirseq
% target seq
% 1 (which zucker version)
% energy
% 4 lines describing the zucker draw
% brzucker_out_data(x) is a struct describing the data for the xth bs
% its feilds are:
% mir id ; utr id; offset; bs_id; mirseq; targetseq; mirlen; targetlen;
% numzuckers; zuckers;
% zuckers{jj} is again a struct with the feilds:
% energy; 4 lines of zucker draw
% numzuckers is how many different zucker folds it found
counter = 0;
while (~feof(fid) & (counter < bs_tot))
    bp1 = [];
    bp2 = [];
    counter = counter + 1;
    tt = fscanf(fid,'%d\n');
    od(counter).bs_id = tt(1);
    od(counter).mirseq = fgetl(fid);
    this_mirlen = length(od(counter).mirseq);
    od(counter).mirlen = this_mirlen;
    od(counter).targetseq = fgetl(fid);
    this_targetlen = length(od(counter).targetseq);
    od(counter).targetlen = this_targetlen;
    nz = 0;
    next_line = fgetl(fid);
    new_bs = 0;
    while (new_bs==0)
        nz = nz+1;
        this_z.version = str2double(next_line);
    end
end

```

```

    e = str2double(fgetl(fid));
    this_z.energy = e;
    line1 = fgetl(fid);
    line2 = fgetl(fid);
    line3 = fgetl(fid);
    line4 = fgetl(fid);
    this_z.draw_line1 = line1;
    this_z.draw_line2 = line2;
    this_z.draw_line3 = line3;
    this_z.draw_line4 = line4;
    od(counter).zukers(nz) = this_z;
    next_line = fgetl(fid);
    if(strcmp(next_line,'|'))
        new_bs = 1;
    end
end
end
od(counter).numzukers = nz;
end
brzucker_out_data = od;
function brzucker_out_data = raed_brzucker(fid,bs_tot)
% function brzucker_out_data = raed_brzucker(fid,bs_tot)
% reads output from Baraks brzucker program. raeds bs_tot binding sites at a time
% format of file:
% for each candidate binding site:
% > ofir's internal bs_id
% mirseq
% target seq
% 1 (which zucker version)
% energy
% 4 lines describing the zucker draw
% brzucker_out_data(x) is a struct describing the data for the xth bs
% its feilds are:
% mir id ; utr id; offset; bs_id; mirseq; targetseq; mirlen; targetlen;
% numzukers; zukers;
% zukers{}} is again a struct with the feilds:
% energy; 4 lines of zucker draw
% numzukers is how many different zucker folds it found
counter = 0;
while (~feof(fid) & (counter < bs_tot))
    bp1 = [];
    bp2 = [];
    counter = counter + 1;
    tt = fscanf(fid,'%d\n');
    od(counter).bs_id = tt(1);
    od(counter).mirseq = fgetl(fid);
    this_mirlen = length(od(counter).mirseq);
    od(counter).mirlen = this_mirlen;
    od(counter).targetseq = fgetl(fid);
    this_targetlen = length(od(counter).targetseq);
    od(counter).targetlen = this_targetlen;

```

```
nz = 0;
next_line = fgetl(fid);
new_bs = 0;
while (new_bs==0)
    nz = nz+1;
    this_z.version = str2num(next_line);
    e = str2num(fgetl(fid));
    this_z.energy = e;
    line1 = fgetl(fid);
    line2 = fgetl(fid);
    line3 = fgetl(fid);
    line4 = fgetl(fid);
    this_z.draw_line1 = line1;
    this_z.draw_line2 = line2;
    this_z.draw_line3 = line3;
    this_z.draw_line4 = line4;
    od(counter).zukers(nz) = this_z;
    next_line = fgetl(fid);
    if(strcmp(next_line,'|'))
        new_bs = 1;
    end
end
od(counter).numzukers = nz;
end
brzucker_out_data = od;
```

```

function [xs,ys,yp2,yp2] = analyse_errors_bins2(pos_estimated,score,pos, endbulges,N)
% measure the distribution of erros
if length(pos_estimated) ~= length(score)
    error('pos_estimated and score not compatible');
end
if length(pos_estimated) ~= length(pos)
    error('pos_estimated and pos not compatible');
end
if length(pos_estimated) ~= length(endbulges)
    error('pos_estimated and endbulges size not compatible');
end
if nargin == 4
    N = 6;
end
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_disth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)-1
    l = find(score <= thresh(i) & score >= thresh(i+1));
    if ~isempty(l)
        count = count + 1;
        midbin(count) = mean(score(l));
        accuracy(count) = sum(pos_estimated(l) == pos(l))/length(l);

        J1 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 1);
        correct_side_dist1(count) = length(J1)/length(l);
        J2 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 2);
        correct_side_dist2(count) = length(J2)/length(l);
        J3 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 3);
        correct_side_dist3(count) = length(J3)/length(l);
        Jh = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) > 3);
        correct_side_disth(count) = length(Jh)/length(l);

        wrong_side(count) = sum(1-correct_side(l))/length(l);

        fraction(count) = length(l)/N;
    else
        count = count+1;
        midbin(count) = NaN;;
    end
end

```

```

    accuracy(count) = NaN;
    correct_side_dist1(count) = NaN;
    correct_side_dist2(count) = NaN;
    correct_side_disth(count) = NaN;
    wrong_side(count) = NaN;
    fraction(count) = NaN;
end
end
acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
acc3 = accuracy + correct_side_dist1 + correct_side_dist2 + correct_side_dist3;
hold on
plot(midbin, acc3,'y','linewidth',2)
plot(midbin, acc2,'g','linewidth',2)
plot(midbin, acc1,'r','linewidth',2)
plot(midbin, accuracy,'b','linewidth',2)
plot(midbin, wrong_side,'k','linewidth',2)
plot(midbin,fraction,'c','linewidth',2)
legend('dist \leq 3', 'dist \leq 2', 'dist \leq 1', 'precise', 'wrong side',2);
plot(midbin, acc3,'dy')
plot(midbin, acc2,'*g')
plot(midbin, acc1,'or')
plot(midbin, accuracy,'bd')
plot(midbin, wrong_side,'kv')
xlabel('bin');
%axis([min(midbin)-1 max(midbin)+1 0 1])
[ry,yp2,mass,xp2,newy,pos] = isotonic_regression(midbin,acc2);
[ry,ys,mass,xs,newy,pos] = isotonic_regression(midbin,1-wrong_side);
returnfunction [x,ys,yp2,yp1,yp0] = analyse_errors_bins3(pos_estimated,score,pos, endbulges,N)
% measure the distribution of erros
if length(pos_estimated) ~= length(score)
    error('pos_estimated and score not compatible');
end
if length(pos_estimated) ~= length(pos)
    error('pos_estimated and pos not compatible');
end
if length(pos_estimated) ~= length(endbulges)
    error('pos_estimated and endbulges size not compatible');
end
if nargin == 4
    N = 6;
end
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_disth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);

```



```

count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1)))); %one for correct side estimate
end
for i = 1:length(thresh)-1
    I = find(score <= thresh(i) & score >= thresh(i+1));
    if ~isempty(I)
        count = count + 1;
        midbin(count) = mean(score(I));
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        J3 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 3);
        correct_side_dist3(count) = length(J3)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 3);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
        midbin(count) = NaN;;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
        correct_side_dsth(count) = NaN;
        wrong_side(count) = NaN;
        fraction(count) = NaN;
    end
end
acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
acc3 = accuracy + correct_side_dist1 + correct_side_dist2 + correct_side_dist3;
hold on
plot(midbin, acc3,'y','linewidth',2)
plot(midbin, acc2,'g','linewidth',2)
plot(midbin, acc1,'r','linewidth',2)
plot(midbin, accuracy,'b','linewidth',2)
plot(midbin, wrong_side,'k','linewidth',2)
plot(midbin,fraction,'c','linewidth',2)
legend('dist \leq 3', 'dist \leq 2', 'dist \leq 1', 'precise', 'wrong side',2);
plot(midbin, acc3,'dy')
plot(midbin, acc2,'*g')
plot(midbin, acc1,'or')

```

```

plot(midbin, accuracy,'bd')
plot(midbin, wrong_side,'kv')
xlabel('bin');
%axis([min(midbin)-1 max(midbin)+1 0 1])
[ry,yp2,mass,xp2,newy,pos] = isotonic_regression(midbin,acc2);
[ry,yp1,mass,xp1,newy,pos] = isotonic_regression(midbin,acc1);
[ry,yp0,mass,xp0,newy,pos] = isotonic_regression(midbin,accuracy);
[ry,ys,mass,xs,newy,pos] = isotonic_regression(midbin,1-wrong_side);
x=xs;
returnfunction res = analyse_errors_perc(pos_estimated,score,pos, endbulges)
%analyse_errors_perc(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
N = 100;
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)
    I = find(score >= thresh(i));
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        J3 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 3);
        correct_side_dist3(count) = length(J3)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 3);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
    end
end

```

```

    correct_side_dsth(count) = NaN;
    wrong_side(count) = NaN;
    fraction(count) = NaN;
end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
acc3 = accuracy + correct_side_dist1 + correct_side_dist2 + correct_side_dist3;
%clf
hold on

plot(perc, acc3,'y','linewidth',2)
plot(perc, acc2,'g','linewidth',2)
plot(perc, acc1,'r','linewidth',2)
plot(perc, accuracy,'b','linewidth',2)
plot(perc, wrong_side,'k','linewidth',2)
plot(perc, thresh,'c','linewidth',2)
legend('dist \leq 3','dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'threshold',2);
xlabel('percentage');
axis([0 100 0 1]);

%keyboard
%prepare result
N = length(accuracy);
res = [accuracy(N), acc1(N), acc2(N), acc3(N), 1-wrong_side(N), acc2(round(0.2*N))];
returnfunction analyse_errors_perc_2preds(pos_estimated,score,pos, endbulges,decide_by,pred_side)
%analyse_errors_perc(pos_estimated,score,pos, endbulges)
%pos_est and score are 2 cols (a pred for each arm with its score)
if(~exist('decide_by'))
    decide_by = 0;
end
if(decide_by == 1) % decide on prediction using real mirside
    for i=1:length(pos)
        lb = find(endbulges{i});
        eb_begin = lb(1);
        eb_end = lb(end);
        mirside = (pos(i)<eb_begin); % mirside=1 if mir is on arm5, 0 if on arm3.
        if(mirside) % arm5
            pos_est_arm(i) = pos_estimated(i,1);
            score_arm(i) = score(i,1);
        else
            pos_est_arm(i) = pos_estimated(i,2);
            score_arm(i) = score(i,2);
        end
    end
end
elseif(decide_by == 0) % decide by best score
    for i=1:length(pos)
        if(score(i,1)>score(i,2))
            pos_est_arm(i) = pos_estimated(i,1);

```

```

        score_arm(i) = score(i,1);
    else
        pos_est_arm(i) = pos_estimated(i,2);
        score_arm(i) = score(i,2);
    end
end
elseif(decide_by == 2) % decide by predicted side
    if(~exist('pred_side'))
        error('must give a predicted side for this option')
    end
    for i=1:length(pos)
        if(pred_side(i)==1) % arm5 predicted
            pos_est_arm(i) = pos_estimated(i,1);
            score_arm(i) = score(i,1);
        else
            pos_est_arm(i) = pos_estimated(i,2);
            score_arm(i) = score(i,2);
        end
    end
end
end
analyse_errors_perc(pos_est_arm,score_arm,pos,endbulges);
function res = analyse_errors_perc_noplot(pos_estimated,score,pos, endbulges)
%analyse_errors_perc(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
N = 100;
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_disth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)
    l = find(score >= thresh(i));
    if ~isempty(l)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(l) == pos(l))/length(l);

        J1 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 1);
        correct_side_dist1(count) = length(J1)/length(l);
        J2 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 2);
        correct_side_dist2(count) = length(J2)/length(l);
        Jh = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) > 2);
    end
end

```

```

correct_side_dsth(count) = length(Jh)/length(I);

wrong_side(count) = sum(1-correct_side(I))/length(I);

fraction(count) = length(I)/N;
else
    count = count+1;
    accuracy(count) = NaN;
    correct_side_dist1(count) = NaN;
    correct_side_dist2(count) = NaN;
    correct_side_dsth(count) = NaN;
    wrong_side(count) = NaN;
    fraction(count) = NaN;
end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
N = length(accuracy);
res = [accuracy(N), acc1(N), acc2(N), 1-wrong_side(N), acc2(round(0.2*N))];
returnfunction analyse_errors_thresh(pos_estimated,score,pos, endbulges,Np)
%analyse_errors_thresh(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
if max(score) > 1
    mxscore = max(score);
else
    mxscore = 1;
end
if min(score) < 0
    mnscore = min(score);
else
    mnscore = 0;
end
if(~exist('Np'))
    Np = 500;
end
dth = (mxscore- mnscore)/Np;
thresh = mnscore:dth:mxscore;
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate

```

```

end
for i = 1:length(thresh)
    I = find(score >= thresh(i));
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 2);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
        correct_side_dsth(count) = NaN;
        wrong_side(count) = NaN;
        fraction(count) = NaN;
    end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
clf
hold on

plot(thresh, acc2,'g')
plot(thresh, acc1,'r')
plot(thresh, accuracy,'b')
plot(thresh, wrong_side,'k')
plot(thresh, fraction,'c')
legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'fraction');
xlabel('threshold');
%keyboard
returnfunction [thresh,acc2,captures] = analyse_errors_thresh_B(pos_estimated,score,pos, endbulges,thresh)
%analyse_errors_thresh_B(pos_estimated,score,pos, endbulges,thresh)
% receives the vector thresh
% measure the distribution of erros
if max(score) > 1
    mxscore = max(score);
else
    mxscore = 1;
end

```

```

end
if min(score) < 0
    mnscore = min(score);
else
    mnscore = 0;
end
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1))))); %one for correct side estimate
end
for i = 1:length(thresh)
    l = find(score >= thresh(i));
    captures(i) = length(l);
    if ~isempty(l)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(l) == pos(l))/length(l);

        J1 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 1);
        correct_side_dist1(count) = length(J1)/length(l);
        J2 = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) == 2);
        correct_side_dist2(count) = length(J2)/length(l);
        Jh = find(correct_side(l) & abs(pos(l)- pos_estimated(l)) > 2);
        correct_side_dsth(count) = length(Jh)/length(l);

        wrong_side(count) = sum(1-correct_side(l))/length(l);

        fraction(count) = length(l)/N;
    else
        count = count+1;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
        correct_side_dsth(count) = NaN;
        wrong_side(count) = NaN;
        fraction(count) = NaN;
    end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;

```

```

hold on
plot(thresh, acc2,'g-o','linewidth',2)
plot(thresh, acc1,'r-o','linewidth',2)
plot(thresh, accuracy,'b-o','linewidth',2)
plot(thresh, wrong_side,'k-o','linewidth',2)
plot(thresh, fraction,'c-o','linewidth',2)
legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'fraction');
xlabel('threshold');
%keyboard
returnfunction [thresh,captures,acc2,acc1,accuracy,correctside] = ...
    analyse_errors_thresh_C(pos_estimated,score,pos, endbulges,thresh)
% [thresh,captures,acc2,acc1,accuracy,correctside] = analyse_errors_thresh_C(pos_estimated,score,pos,
endbulges,thresh)
% receives the vector thresh
% measure the distribution of erros
if max(score) > 1
    mxscore = max(score);
else
    mxscore = 1;
end
if min(score) < 0
    mnscore = min(score);
else
    mnscore = 0;
end
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1)))); %one for correct side estimate
end
for i = 1:length(thresh)
    I = find(score >= thresh(i));
    captures(i) = length(I);
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 2);
        correct_side_dsth(count) = length(Jh)/length(I);
    end
end

```



```

wrong_side(count) = sum(1-correct_side(l))/length(l);

fraction(count) = length(l)/N;
else
    count = count+1;
    accuracy(count) = NaN;
    correct_side_dist1(count) = NaN;
    correct_side_dist2(count) = NaN;
    correct_side_dsth(count) = NaN;
    wrong_side(count) = NaN;
    fraction(count) = NaN;
end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
correctside = 1-wrong_side;

hold on
plot(thresh, acc2,'g-o','linewidth',2)
plot(thresh, acc1,'r-o','linewidth',2)
plot(thresh, accuracy,'b-o','linewidth',2)
plot(thresh, wrong_side,'k-o','linewidth',2)
plot(thresh, fraction,'c-o','linewidth',2)
legend('dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'fraction');
xlabel('threshold');
%keyboard
returnfunction mfe = anti_inds_to_mfe(anti_inds)
% anti_inds holds for each nuc in the seq what is the index of
% the nuc across from it where the 0 means unpaired (this is returned by read_structure_withanti).
% returns mfe which is the structure in the format of rnafold, i.e. only base pairs:
% mfe is a 2 col matrix, the first being the bases on arm5 which are paired and the second
% their corresponding pairs
if(~iscell(anti_inds))
    mfe = get_mfe(anti_inds);
    return;
end
for i=1:length(anti_inds)
    mfe{i} = get_mfe(anti_inds{i});
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function mfe = get_mfe(ai)
bps=0;
for i=1:length(ai)
    if(ai(i))
        if(i>ai(i))
            return

```

```

    end
    bps = bps+1;
    mfe(bps,1) = i;
    mfe(bps,2) = ai(i);
end
end
function [sum_in_win, sum_in_win_mfe, sum_out, sum_out_mfe, faulty] = ...
    base_pairing(pal_len, bp_prob, mfe, winstart5, win_len)
% function [sum_in_win, sum_in_win_mfe, sum_out, sum_out_mfe, faulty] = ...
%   base_pairing(pal_len, bp_prob, mfe, winstart5, win_len)
% pal_len is length of palindrom
% bp_prob is the base pairing prob matrix which has 3 cols:
% 5side index, 3side index, prob to be paired
% mfe has the pairs in the min free energy drawing
% winstart5 is the position of the start of the window in question
% win_len is its length
% sum_in_win is the sum of the bp probs of all pairs involving a base
% in the designated window normalized by win_len
% sum_in_win_mfe is the sum of the bp probs of all pairs appearing
% in the mfe structure and involving a base in the window. this is
% normalized by the number of base pairs appearing in the mfe structure
% within the window (if only one folding possible sum_in_win_mfe=1).
% sum_out is like sum_in only all bases not in window. normalized by
% ((pal_len+eb_len)/2 - win_len).
% sum_out_mfe is like sum_in_win_mfe only for all bp not in window.
% analogous normalization.
% if window is illegal, returns faulty=1 and NAN for other values
% also note that no check is made on winstart5 and win_len being positive (which they must) - beware!
n_pairs = size(bp_prob,1);
n_mfe_pairs = size(mfe,1);
arm5 = mfe(:,1);
arm3 = mfe(:,2);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1; % num nucs in end bulge
win_inds = [winstart5:winstart5+win_len-1];
if(any(intersect(win_inds,[eb_start:eb_end])) | win_inds(end)>pal_len)
    faulty = 1;
    sum_in_win = NaN;
    sum_in_win_mfe = NaN;
    sum_out = NaN;
    sum_out_mfe = NaN;
    disp('WINDOW IS ILLEGAL. RETURNING FAULTY=1. ');
    disp(['window has ' num2str(length(intersect(win_inds,[eb_start:eb_end]))) ' nucs in endloop']);
    return
end
sum_in_win = 0;
sum_in_win_mfe = 0;
sum_out = 0;
sum_out_mfe = 0;

```

```

faulty = 0;
n_mfe_pairs_inwin = 0;
for i=1:n_pairs
    side5 = bp_prob(i,1);
    side3 = bp_prob(i,2);
    if(ismembc(side5,win_inds) | ismembc(side3,win_inds))
        sum_in_win = sum_in_win + bp_prob(i,3);
        if(ismember([side5,side3],mfe,'rows'))
            sum_in_win_mfe = sum_in_win_mfe + bp_prob(i,3);
            n_mfe_pairs_inwin = n_mfe_pairs_inwin + 1;
        end
    else
        sum_out = sum_out + bp_prob(i,3);
        if(ismember([side5,side3],mfe,'rows'))
            sum_out_mfe = sum_out_mfe + bp_prob(i,3);
        end
    end
end
% normalization
sum_in_win = sum_in_win/win_len;
sum_in_win_mfe = sum_in_win_mfe/n_mfe_pairs_inwin;
sum_out = sum_out/((pal_len-eb_len)/2 - win_len);
sum_out_mfe = sum_out_mfe/(n_mfe_pairs-n_mfe_pairs_inwin);
function [sum_in_win, sum_out, faulty] = ...
    base_pairing_nomfe(pal_len, bp_prob, mfe, winstart5, win_len)
% function [sum_in_win, sum_out, faulty] = ...
%   base_pairing(pal_len, bp_prob, mfe, winstart5, win_len)
% same as base_pairing but only computes these outputs (much faster)
n_pairs = size(bp_prob,1);
n_mfe_pairs = size(mfe,1);
arm5 = mfe(:,1);
arm3 = mfe(:,2);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1; % num nucs in end bulge
win_inds = [winstart5:winstart5+win_len-1];
if(any(intersect(win_inds,[eb_start:eb_end])) | win_inds(end)>pal_len)
    faulty = 1;
    sum_in_win = NaN;
    sum_out = NaN;
    disp('WINDOW IS ILLEGAL. RETURNING FAULTY=1. ');
    disp(['window has ' num2str(length(intersect(win_inds,[eb_start:eb_end]))) ' nucs in endloop']);
    return
end
sum_in_win = 0;
sum_out = 0;
faulty = 0;
n_mfe_pairs_inwin = 0;
for i=1:n_pairs
    side5 = bp_prob(i,1);

```

```

side3 = bp_prob(i,2);
if(ismembc(side5,win_inds) | ismembc(side3,win_inds))
    sum_in_win = sum_in_win + bp_prob(i,3);
else
    sum_out = sum_out + bp_prob(i,3);
end
end
% normalization
sum_in_win = sum_in_win/win_len;
sum_out = sum_out/((pal_len-eb_len)/2 - win_len);
function [sum_in_win, sum_in_win_mfe, sum_out, sum_out_mfe, faulty] = ...
    base_pairing(pal_len, bp_prob, mfe, wstart5, win_len)
% function [sum_in_win, sum_in_win_mfe, sum_out, sum_out_mfe, faulty] = ...
%   base_pairing(pal_len, bp_prob, mfe, wstart5, win_len)
% pal_len is length of palindrom
% bp_prob is the base pairing prob matrix which has 3 cols:
% 5side index, 3side index, prob to be paired
% mfe has the pairs in the min free energy drawing
% wstart5 is the position of the start of the window in question
% win_len is its length
% sum_in_win is the sum of the bp probs of all pairs involving a base
% in the designated window normalized by win_len
% sum_in_win_mfe is the sum of the bp probs of all pairs appearing
% in the mfe structure and involving a base in the window. this is
% normalized by the number of base pairs appearing in the mfe structure
% within the window (if only one folding possible sum_in_win_mfe=1).
% sum_out is like sum_in only all bases not in window. normalized by
% ((pal_len-eb_len)/2 - win_len).
% sum_out_mfe is like sum_in_win_mfe only for all bp not in window.
% analogous normalization.
% if window is illegal, returns faulty=1 and NaN for other values
% also note that no check is made on wstart5 and win_len being positive (which they must) - beware!
n_pairs = size(bp_prob,1);
n_mfe_pairs = size(mfe,1);
arm5 = mfe(:,1);
arm3 = mfe(:,2);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1; % num nucs in end bulge
win_inds = [wstart5:wstart5+win_len-1];
if(any(intersect(win_inds,[eb_start:eb_end])) | win_inds(end)>pal_len)
    faulty = 1;
    sum_in_win = NaN;
    sum_in_win_mfe = NaN;
    sum_out = NaN;
    sum_out_mfe = NaN;
    disp('WINDOW IS ILLEGAL. RETURNING FAULTY=1. ');
    disp(['window has ' num2str(length(intersect(win_inds,[eb_start:eb_end]))) ' nucs in endloop']);
    return
end
end

```

```

sum_in_win = 0;
sum_in_win_mfe = 0;
sum_out = 0;
sum_out_mfe = 0;
faulty = 0;
n_mfe_pairs_inwin = 0;
for i=1:n_pairs
    side5 = bp_prob(i,1);
    side3 = bp_prob(i,2);
    if(ismember(side5,win_inds) | ismember(side3,win_inds))
        sum_in_win = sum_in_win + bp_prob(i,3);
        if(ismember([side5,side3],mfe,'rows'))
            sum_in_win_mfe = sum_in_win_mfe + bp_prob(i,3);
            n_mfe_pairs_inwin = n_mfe_pairs_inwin + 1;
        end
    else
        sum_out = sum_out + bp_prob(i,3);
        if(ismember([side5,side3],mfe,'rows'))
            sum_out_mfe = sum_out_mfe + bp_prob(i,3);
        end
    end
end
end
% normalization
sum_in_win = sum_in_win/win_len;
sum_in_win_mfe = sum_in_win_mfe/n_mfe_pairs_inwin;
sum_out = sum_out/((pal_len-eb_len)/2 - win_len);
sum_out_mfe = sum_out_mfe/(n_mfe_pairs-n_mfe_pairs_inwin);
function [sum_in_win, sum_in_win_mfe, sum_out, sum_out_mfe, faulty] = ...
    base_pairing2(pal_len, bp_prob, mfe, winstart5, win_len)
% function [sum_in_win, sum_in_win_mfe, sum_out, sum_out_mfe, faulty] = ...
%     base_pairing2(pal_len, bp_prob, mfe, winstart5, win_len)
% see base_pairing but here no normalization
n_pairs = size(bp_prob,1);
n_mfe_pairs = size(mfe,1);
arm5 = mfe(:,1);
arm3 = mfe(:,2);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1; % num nucs in end bulge
win_inds = [winstart5:winstart5+win_len-1];
if(any(intersect(win_inds,[eb_start:eb_end])) | win_inds(end)>pal_len)
    faulty = 1;
    sum_in_win = NaN;
    sum_in_win_mfe = NaN;
    sum_out = NaN;
    sum_out_mfe = NaN;
    disp('WINDOW IS ILLEGAL. RETURNING FAULTY=1.');
```

```

sum_in_win = 0;
sum_in_win_mfe = 0;
sum_out = 0;
sum_out_mfe = 0;
faulty = 0;
n_mfe_pairs_inwin = 0;
for i=1:n_pairs
    side5 = bp_prob(i,1);
    side3 = bp_prob(i,2);
    if(ismembc(side5,win_inds) | ismembc(side3,win_inds))
        sum_in_win = sum_in_win + bp_prob(i,3);
        if(ismember([side5,side3],mfe,'rows'))
            sum_in_win_mfe = sum_in_win_mfe + bp_prob(i,3);
            n_mfe_pairs_inwin = n_mfe_pairs_inwin + 1;
        end
    else
        sum_out = sum_out + bp_prob(i,3);
        if(ismember([side5,side3],mfe,'rows'))
            sum_out_mfe = sum_out_mfe + bp_prob(i,3);
        end
    end
end
function [y, df] = chi2(table)
%[y, df] = chi2(table)
%calculate chi2 valuse for m*n table, with m,n>1
n = sum(table(:));
sum2 = sum(table,1);
sum1 = sum(table,2);
% calculate the expected vals , assuming independence
ex = 0;
for i1 = 1:size(table,1);
    for i2 = 1:size(table,2)
        ex(i1,i2) = sum1(i1) *sum2(i2)/n;
    end
end
if any(sum1 == 0) | any(sum2 == 0)
    y = NaN;
else
    y = sum(sum((ex-table).^2./ex));
end
df = (size(table,1)-1)*(size(table,2)-1);
return
function T=clusterize_prototype(seqs,maxd)
%T=clusterize_prototype(seqsd,maxd)
%clusterize by edist. all examples within cluster have edist < maxd.
%pick one prototype from each cluster
%T(i) = 1 if example i is to be used. T(i) = 0 if example i is to be ignored.
if ~all(isletter(seqs{1}))
    for i = 1:length(seqs)
        seqs{i} = int2nuc(seqs{i});
    end
end

```

```

    end
end
if length(seqs{1}) > 25
    disp('sequence is longer than 25. press enter to continue');
    pause
end
nseq=length(seqs);
%maxseq=ceil(nseq/Nc);
dij=zeros((nseq-1)*nseq/2,3);
count = 0;
for i=1:nseq-1
    for j=i+1:nseq
        count = count+1;
        dij(count,:)=editD(seqs{i},seqs{j}),i,j];
    end
end
sdij=sortrows(dij);
npair=length(sdij);
for i=1:nseq
    ss{i}=i;
end
iseq=[1:nseq];
s2g=iseq;
ng=ones(nseq,1);
Nc=0;
useg=[];
for i=1:npair
    gid=s2g(sdij(i,[2 3]));
    if ((diff(gid)~=0) & (sdij(i,1)<maxd))
        g=union(ss{gid});
        ss{gid(1)}=g;
        s2g(g)=gid(1);
        ng(g)=0;
        ng(gid(1))=length(g);
    end
end
end

ii=find(ng>0);
grp={ss{ii}};
T = zeros(1,length(seqs));
rand('state',121);
for i = 1:length(ii)
    s=ss{ii(i)};
    r=ceil(rand*length(s));
    T(s(r)) = 1;
end
return
function grp=clusterize_prototype1(seqs,maxd)
%T=clusterize_prototype1(seqsd,maxd)
%clusterize by edist. all examples within cluster have edist < maxd.

```

```

%grp is a cell array containing the cluster members
if ~all(isletter(seqs{1}))
    for i = 1:length(seqs)
        seqs[i] = int2nuc(seqs{i});
    end
end
if length(seqs{1}) > 25
    disp('sequence is longer than 25. press enter to continue');
    pause
end
nseq=length(seqs);
%maxseq=ceil(nseq/Nc);
dij=zeros(0.5*nseq*(nseq-1),3);
count = 0;
for i=1:nseq-1
    for j=i+1:nseq
        dij(count+1,:)=editD(seqs{i},seqs{j}),i,j];
        count = count+1;
    end
end
sdij=sortrows(dij);
npair=length(sdij);
for i=1:nseq
    ss{i}=i;
end
iseq=[1:nseq];
s2g=iseq;
ng=ones(nseq,1);
Nc=0;
useg=[];
for i=1:npair
    gid=s2g(sdij(i,[2 3]));
    if ((diff(gid)~=0) & (sdij(i,1)<maxd))
        g=union(ss{gid});
        ss{gid(1)}=g;
        s2g(g)=gid(1);
        ng(g)=0;
        ng(gid(1))=length(g);
    end
end
ii=find(ng>0);
grp={ss{ii}};
T = zeros(1,length(seqs));
rand('state',121);
for i = 1:length(ii)
    s=ss{ii(i)};
    r=ceil(rand*length(s));
    T(s(r)) = 1;
end

```



```

return
overhang = 2;
clear set_name;
set_name = 'h104';
load_training_from_mat;
mir_win = get_win_pos_overhang_v1(anti_inds,pos,mirlen,overhang);
num_nan_wins = 0;
num_amb_wins = 0;
for i= 1:length(mir_win)
    w = mir_win{i};
    if(~isstruct(w))
        num_nan_wins = num_nan_wins+1;
    else
        if(w.ambiguous)
            num_amb_wins = num_amb_wins+1;
        end
    end
end
length(mir_win)
num_nan_wins
num_amb_wins
function create_file_for_rnastructure(seq,filename)
if(~isletter(seq(1)))
    seq=int2nuc(seq);
end
pause(1)
fid = fopen(filename,'w');
fprintf(fid,'\n1\n');
for i = 1:length(seq)
    fprintf(fid,seq(i));
end
fprintf(fid,'1\n');
fclose(fid);function h = entropy(p,base)
% function h = entropy(p,base)
% function h = entropy(p)
% computes the entropy of the distribution p in base base
% if no base is given assumes base 2
h = sum(-1*xlog2x(p));
if(nargin==2)
    h = h/log2(base);
end
%%%%%%%%%%

function y = xlog2x(x)
l = 1:length(x);
l0 = find(x==0);
y(l0) = 0;
l1 = setdiff(l,l0);
y(l1) = x(l1).*log2(x(l1));
function [anti_nucs,which_case] = get_anti_nucs(pos,pal_pos_bp,mfe)

```

```

% function anti_nucs = get_anti_nucs(pos,pal_pos_bp,mfe)
% pal_pos_bp is a vector of length pallen which holds the position of the nuc
% in the following format: all bp are numbered from legs by 1,2,3,...
% If a nuc is paired its pos_bp is the number of its bp. If not it is interpolated
% if the nuc is on the end loop pos_bp = 0.
% pos is the real position.
% anti_nucs gives the pos of the nuc across from pos. in some cases gives a few options.
% which_case is a string signaling the case:
% end_loop - pos sits on endloop, anti_nucs=nan in this case.
% bp - base paired
% equal_bulge
% small_bulge
% large_bulge
% non_sym_bulge
% how to determine across:
% if paired - obvious
% if on bulge and across bulge of same length, corresponding on anti bulge
% if on bulge smaller than antibulge: all options that don't cross
% if on bulge larger than antibulge and antibulge not empty: corresponding to
% all options that dont cross
% if on bulge and no bulge across: to closest bp across(if exactly in middle gives both option)
pallen = length(pal_pos_bp);
eb_start = mfe(end,1)+1;
eb_end = mfe(end,2)-1;
if(intersect([eb_start:eb_end],pos))
    %warning(['get_anti_nucs: pos sits on endloop. returning NAN. (pos = ' num2str(pos) ')']);
    anti_nucs = nan;
    which_case = 'end_loop';
    return;
end
if(pos<1 | pos>pallen)
    %warning(['get_anti_nucs: pos sits outside of pal. returning NAN. (pos = ' num2str(pos) ')']);
    anti_nucs = nan;
    which_case = 'outside pal';
    return;
end
pos_bp = pal_pos_bp(pos); % bp number of nuc in question
mod_pos_bp = mod(pos_bp,1);
if(mod_pos_bp==0) % nuc is paired
    this_pair = mfe(pos_bp,:);
    tt = find(this_pair == pos);
    anti_nucs = this_pair(setdiff([1:2],tt));
    which_case = 'bp';
    return;
end
% from here means nuc is unpaired
pos_side = 2-(pos<eb_start); % 1 for arm5, 2 for arm3.
pos_anti_side = setdiff([1:2],pos_side);
if(pos_side==1)
    my_side_inds = 1:eb_start-1;

```

```

else
    my_side_inds = eb_end+1:pallen;
end
bp_before = pos_bp - mod_pos_bp;
bp_after = bp_before + 1;
if(bp_before>0)
    num_in_my_bulge = abs(mfe(bp_after,pos_side) - mfe(bp_before,pos_side))-1;
    num_in_anti_bulge = abs(mfe(bp_after,pos_anti_side) - mfe(bp_before,pos_anti_side))-1;
else
    num_in_my_bulge = min(mfe(bp_after,pos_side)-1,abs(mfe(bp_after,pos_side)-pallen));
    num_in_anti_bulge = min(mfe(bp_after,pos_anti_side)-1,abs(mfe(bp_after,pos_anti_side)-pallen));
end
if(num_in_my_bulge == num_in_anti_bulge)
    tt = find(pal_pos_bp==pos_bp);
    anti_nucs = setdiff(tt,pos);
    which_case = 'equal_bulge';
    return;
end
my_bulge_vec = linspace(bp_before,bp_after,num_in_my_bulge+2);
my_bulge_vec = my_bulge_vec(2:end-1);
anti_bulge_vec = linspace(bp_before,bp_after,num_in_anti_bulge+2);
anti_bulge_vec = anti_bulge_vec(2:end-1);
my_place = find(my_bulge_vec==pos_bp);
if(num_in_my_bulge < num_in_anti_bulge)
    for i=1:(num_in_anti_bulge-num_in_my_bulge+1)
        tt = find(pal_pos_bp == anti_bulge_vec(my_place+i-1));
        % make sure not finding anything in my_bulge (that is look only in other side):
        anti_nucs(i) = setdiff(tt,my_side_inds);
    end
    which_case = 'small_bulge';
    return;
end
if((num_in_my_bulge > num_in_anti_bulge) & num_in_anti_bulge>0)
    anti_nucs = [];
    for i=1:(num_in_my_bulge-num_in_anti_bulge+1)
        tt = my_place-i+1;
        if(tt>0 & tt<=num_in_anti_bulge)
            ttt = find(pal_pos_bp == anti_bulge_vec(tt));
            % make sure not finding anything in my_bulge (that is look only in other side):
            anti_nucs = [anti_nucs,setdiff(ttt,my_side_inds)];
        end
    end
    which_case = 'large_bulge';
    return;
end
if(num_in_anti_bulge == 0)
    if(mod_pos_bp==0.5)
        anti_nucs(1) = mfe(bp_after,pos_anti_side);
        if(bp_before>0)
            anti_nucs(2) = mfe(bp_before,pos_anti_side);
        end
    end
end

```

```

    end
elseif(mod_pos_bp<0.5 & bp_before>0)
    anti_nucs = mfe(bp_before,pos_anti_side);
else
    anti_nucs = mfe(bp_after,pos_anti_side);
end
which_case = 'non_sym_bulge';
return;
end
% really shouldn't be here
error('terrible mistake... aborting');

```

```

function [energy,mfe] = get_from_ct(ct_file)
% gets the energy and mfe of first zucker fold as outputted from rnastructure
% caution: relies on the very specific format of the out file ct_file - check!
ct_file
fid = fopen(ct_file,'r');
if(fid==-1)
    keyboard
end
line = fgetl(fid);
x = findstr('ENERGY',line);
if isempty(x)
    energy = 0;
    mfe = [];
    fclose(fid);
    return;
end
seqlen = str2num(line(1:x-1));
x = findstr('=',line);
ll = line(x+2:end);
x = findstr(' ',ll);
energy_s = ll(1:x);
energy = str2num(energy_s);
count = 0;
for i=1:seqlen
    line = fgetl(fid);
    v = str2num(line(8:end));
    across = v(3);
    if(across>0 & across<i)
        % already redundant info
        break;
    end
    if(across>0)
        count = count+1;
        mfe(count,1) = i;
        mfe(count,2) = across;
    end
end
end
fclose(fid);

```

```

function pos_bp = get_pos_bp(anti_inds)
% function pos_bp = get_pos_bp(anti_inds)
% pos_bp{i} is a vector of length pallen(i) holding the position of the nuc
% in the following format: all bp are numbered from legs by 1,2,3,...
% If a nuc is paired its pos_bp is the number of its bp. If not it is interpolated
% if the nuc is on the end loop pos_bp = 0
vec_flag = 0;
if(~iscell(anti_inds))
    tt{1} = anti_inds;
    anti_inds = tt;
    vec_flag = 1;
end
for i=1:length(anti_inds)
    ai = anti_inds{i};
    pallen = length(ai);
    mfe = anti_inds_to_mfe(ai);
    this_pos_bp = zeros(1,pallen);
    arm5 = mfe(:,1);
    arm3 = mfe(:,2);
    eb_start = arm5(end)+1;
    eb_end = arm3(end)-1;
    eb_len = eb_end-eb_start+1; % num nucs in end bulge

    this_pos_bp(arm5(1)) = 1;
    this_pos_bp(arm3(1)) = 1;
    d5 = arm5(1)-1;
    for k=1:d5
        this_pos_bp(k) = k/(d5+1);
    end
    d3 = pallen-arm3(1);
    for k=1:d3
        this_pos_bp(arm3(1)+k) = (d3+1-k)/(d3+1);
    end
    for j=2:length(arm5)
        this_pos_bp(arm5(j)) = j;
        this_pos_bp(arm3(j)) = j;
        d5 = arm5(j)-arm5(j-1)-1; %how many nucs in bulge between them
        for k=1:d5
            this_pos_bp(arm5(j-1)+k) = j-1 + k/(d5+1);
        end
        d3 = arm3(j-1)-arm3(j)-1;
        for k=1:d3
            this_pos_bp(arm3(j)+k) = j-1 + (d3+1-k)/(d3+1);
        end
    end
    pos_bp{i} = this_pos_bp;
end
if(vec_flag)
    tt = pos_bp{1};
    pos_bp = tt;
end

```

```

end
function win_mirpos = get_win_pos_v1(mfes,anti_inds,mirpos,mirlen)
% function win_mirpos = get_win_pos(mfes,anti_inds,mirpos,mirlen)
% returns win_mirpos in index of basepair (from legs not loop).
% i.e. mfe(win_mirpos,1) is the nuc pos on the 5 arm
% for mir on arm3 returns the closest bp from its mirpos towards the legs
% for mir on arm5 returns the closest bp from its END (mirpos+mirlen-1) towards the legs
% also towards the legs
for i=1:length(mirpos)
    pos5 = mirpos(i);
    pos3 = pos5+mirlen(i)-1;
    mfe = mfes{i};
    arm5 = mfe(:,1);
    arm3 = mfe(:,2);
    eb_start = arm5(end)+1;
    eb_end = arm3(end)-1;
    eb_len = eb_end-eb_start+1;
    side5 = (pos5<eb_start);
    ai = anti_inds{i};
    is_paired = (ai~=0);
    if(side5)
        k=0;
        while(~is_paired(pos3-k))
            k=k+1;
        end
        win_mirpos(i) = find(arm5==(pos3-k));
    else
        k=0;
        while(~is_paired(pos5+k))
            k=k+1;
        end
        win_mirpos(i) = find(arm3==(pos5+k));
    end
    if isempty(win_mirpos(i)))
        error('get_win_pos: fatal error. aborting.');
```

```

end
end
function win_mirpos = get_win_pos_v2(mfes,anti_inds,mirpos,mirlen)
% function win_mirpos = get_win_pos(mfes,anti_inds,mirpos,mirlen)
% returns win_mirpos in index of basepair (from legs not loop).
% i.e. mfe(win_mirpos,1) is the nuc pos on the 5 arm
% for mir on arm3 returns the closest bp from its mirpos towards the loop
% for mir on arm5 returns the closest bp from its END towards the loop (mirpos+mirlen-1)
% also towards the legs
for i=1:length(mirpos)
    pos5 = mirpos(i);
    pos3 = pos5+mirlen(i)-1;
    mfe = mfes{i};
    arm5 = mfe(:,1);
    arm3 = mfe(:,2);

```

```

eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1;
side5 = (pos5<eb_start);
ai = anti_inds{i};
is_paired = (ai~=0);
if(side5)
    k=0;
    while(~is_paired(pos3+k))
        k=k+1;
    end
    tt = find(arm5==(pos3+k));
    if(tt)
        win_mirpos(i) = tt;
    else
        win_mirpos(i) = nan;
        disp(['mir ' num2str(i) ' intersects with loop - returning win_mirpos nan']);
    end
else
    k=0;
    while(~is_paired(pos5-k))
        k=k+1;
    end
    tt = find(arm3==(pos5-k));
    if(tt)
        win_mirpos(i) = tt;
    else
        win_mirpos(i) = nan;
        disp(['mir ' num2str(i) ' intersects with loop - returning win_mirpos nan']);
    end
end
end
if isempty(win_mirpos(i))
    error('get_win_pos: fatal error. aborting. ');
end
if (ismember(pos5,eb_start:eb_end) | ismember(pos3,eb_start:eb_end))
end
end

function win_mirpos = get_win_pos_v3(mfes,anti_inds,mirpos,mirlen)
% function win_mirpos = get_win_pos_v3(mfes,anti_inds,mirpos,mirlen)
% returns win_mirpos in index of basepair (from legs not loop).
% i.e. mfe(win_mirpos,1) is the nuc pos on the 5 arm
% for mir on arm3 returns the closest bp from its END (mirpos+mirlen-1) towards the LOOP
% for mir on arm5 returns the closest bp from its mirpos towards the LOOP
% also towards the legs
for i=1:length(mirpos)
    pos5 = mirpos(i);
    pos3 = pos5+mirlen(i)-1;
    mfe = mfes{i};
    arm5 = mfe(:,1);
    arm3 = mfe(:,2);

```

```

eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1;
side5 = (pos5<eb_start);
ai = anti_inds{i};
is_paired = (ai~=0);
if(side5)
    k=0;
    while(~is_paired(pos5+k))
        k=k+1;
    end
    win_mirpos(i) = find(arm5==(pos5+k));
else
    k=0;
    while(~is_paired(pos3-k))
        k=k+1;
    end
    win_mirpos(i) = find(arm3==(pos3-k));
end
if isempty(win_mirpos(i)))
    error('get_win_pos: fatal error. aborting.');
```

```

end
end

function get_zuker_draw_by_number(drawfile,n)
% function get_zuker_draw_by_number(drawfile,n)
% given a file of zuker draws and a number, spills on the workspace the
% zuker draw number n in the file
fid = fopen(drawfile,'r');
ind = 0;
found_flag = 0;
while (~feof(fid) & found_flag==0)
    ind = ind + 1; % index going to read now
    if(ind==n)
        found_flag==1;
        disp('.')
        for i = 1:4
            line = fgetl(fid);
            disp(line);
        end
        disp('.');
    else
        for i = 1:4
            line = fgetl(fid);
        end
    end
end
end

fclose(fid);function strseq = int2nuc(intseq, ncase)
%strseq = int2nuc(intseq, ncase)
%convert a sequence of '1 2 3 4' into 'A C T G' or 'a c t g'
% ncase = uppercase | lowercase

```



```

if(isletter(intseq(1)))
    strseq = intseq;
    return;
end
if nargin == 1
    ncase = 'uppercase';
end
if strcmp(ncase,'uppercase')
    nucs = 'ACTG';
elseif strcmp(ncase,'lowercase')
    nucs = 'actg';
end
strseq = char(size(intseq));
for i = 1:length(intseq)
    strseq(i) = nucs(intseq(i));
end
return
function [yside, yprec2] = interpolate_prob_new(score, fitfile);
%[yside, yprec2] = interpolate_prob_new(score, fitfile);
% load the parameters for interpolation
load(fitfile);
%interpolate
yside = interp1(xs,ys,score,'linear');
yprec2 = interp1(xp2,yp2,score,'linear');
% extrapolate if necessary
if(min(xs)==xs(1)) % x is increasing
    yside(score<xs(1)) = ys(1);
    yprec2(score<xp2(1)) = yp2(1);
    yside(score>xs(end)) = ys(end);
    yprec2(score>xp2(end)) = yp2(end);
else % x is decreasing
    yside(score>xs(1)) = ys(1);
    yprec2(score>xp2(1)) = yp2(1);
    yside(score<xs(end)) = ys(end);
    yprec2(score<xp2(end)) = yp2(end);
end
returnfunction [yside, yprec2] = interpolate_prob_new_txt(score, fitfile);
%[yside, yprec2] = interpolate_prob_new(score, fitfile);
% fitfile is a text file
% load the parameters for interpolation
fid = fopen(fitfile,'r');
while ~feof(fid)
    line = fgetl(fid);
    if ~isstr(line), break, end;
    eval(line)
end
fclose(fid);
%interpolate
yside = interp1(xs,ys,score,'linear');
yprec2 = interp1(xp2,yp2,score,'linear');

```

```

% extrapolate if necessary
if(min(xs)==xs(1)) % x is increasing
    yside(score<xs(1)) = ys(1);
    yprec2(score<xp2(1)) = yp2(1);
    yside(score>xs(end)) = ys(end);
    yprec2(score>xp2(end)) = yp2(end);
else % x is decreasing
    yside(score>xs(1)) = ys(1);
    yprec2(score>xp2(1)) = yp2(1);
    yside(score<xs(end)) = ys(end);
    yprec2(score<xp2(end)) = yp2(end);
end

returnfunction [ry,ry_unique,mass,newx,newy,pos] = isotonic_regression(x,y)
% function [ry,ry_unique,mass,newx,neyy,pos] = isotonic_regression(x,y)
% first uniques x and attaches to it a y which the average of all y's
% attached to same x value (returns these new x and y).
% Also returns the "mass" of each point, so if a few points had the
% same x they are now lumped to one point, whose newy is the mean of
% the original ys.
% ry_unique is the regression of the "uniqued points". ry retains the
% dimensionality of the data.
% pos is such that sort(x)=newx(pos)
% (newx,ry_unique) are the new points. i.e they are sorted x's s.t. each x
% has one point y attached which is monotonous (the result of the IR).
% short short description: after running this function use as the new vectors
% newx and ry_unique
x=x(:); y=y(:);
oldx=x;
oldy=y;
if(length(x)~=length(y))
    disp('x and y must be of same length');
    return;
end
% sort the data according to x
[x,sortind]=sort(x);
y=y(sortind);
% first find avg of y's corresponding to the same x:
[x ndx pos]=unique(x);
mass=diff([0;ndx]); % uses the fact that x is sorted!!!!
counter=1;
for t=1:length(x)
    y(t)=mean(y(counter:counter+mass(t)-1));
    counter=counter+mass(t);
end
y(length(x)+1:length(y))=[];
ry=zeros(size(x));
ry(1)=y(1);
for i=2:length(x)

    ry(i)=y(i);

```

```

j=i;
while(j>1)
    if(ry(j)>=ry(j-1)) break; end
    newy=sum(mass(j-1:i).*ry(j-1:i))/sum(mass(j-1:i));
    ry(j-1:i)=newy;
    j=j-1;
end % while

end % i loop
ry_unique=ry;
ry=zeros(size(oldy));
counter=1;
for t=1:length(ry_unique)
    for j=1:mass(t)
        rytmp(counter)=ry_unique(t);
        counter=counter+1;
    end
end
ry(sortind)=rytmp;
newx=x;
newy=y;
data_dir = 'data_baseline_13_4';
%data_dir = 'data_baseline_15_5';
%data_dir = 'data_baseline_15_5\edist_above_87';
if(~exist('set_name'))
    %set_name = 'edist_above_87';
    set_name = 'h121';
end
if ~exist('randomize')
    randomize = 0;
end
if ~exist('remove_duplicate_mirs')
    remove_duplicate_mirs = 0;
end
palfile = ['c:\rosetta\' data_dir \'zucker_draw_' set_name '.txt'];
[seqs,anti_inds,bulges1,bulges2,endbulges,seq_id] = read_structure_withanti(palfile);
mirseqfile = ['c:\rosetta\' data_dir \'dicerseq_' set_name '.txt'];
[mirseqs,mirlen] = read_seq(mirseqfile);
pos = locate_dicer(mirseqs,seqs);
if randomize
    rand('state',sum(100*clock));
    disp('performing randomized permutation');
    l = randperm(length(seqs));
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    anti_inds = anti_inds(l);
    endbulges = endbulges(l);
    mirlen = mirlen(l);
    pos = pos(l);
    seq_id = seq_id(l);
end

```

```

seqs = seqs(l);
mirseqs = mirseqs(l);
end
if remove_duplicate_mirs
    disp('removing duplicate mirs');
    D = zeros(length(seqs),1); % list of duplicate mirs
    for i = 1:length(seqs)
        for j = i+1:length(seqs)
            if length(mirseqs{j}) == length(mirseqs{i})
                if all(mirseqs{j} == mirseqs{i})
                    D(j) = 1;
                    break;
                end
            end
        end
    end
end
I = find(D);
bulges1(I) = [];
bulges2(I) = [];
anti_inds(I) = [];
endbulges(I) = [];
mirlen(I) = [];
pos(I) = [];
seq_id(I) = [];
seqs(I) = [];
mirseqs(I) = [];
end
lend=mirlen; % some applications use lend and not mirlen.
data_dir = 'data_baseline_15_5';
if(~exist('set_name'))
    set_name = 'hmdc294';
end
filename = ['c:\rosetta\' data_dir \vars_\' set_name]
load(filename);
mirlen = lend;if(~exist('d'))
    d = 'h121';
end
if ~exist('randomize')
    randomize = 1;
end
if ~exist('remove_duplicate_mirs')
    remove_duplicate_mirs = 1;
end
palseqfile = ['c:\rosetta\data_baseline_13_4\palseq_' d '.txt'];
[seqs,pallen] = read_seq(palseqfile);
mirseqfile = ['c:\rosetta\data_baseline_13_4\dicerseq_' d '.txt'];
[mirseqs,mirlen] = read_seq(mirseqfile);
pos = locate_dicer(mirseqs,seqs);
palmfefeile = ['c:\rosetta\data_baseline_13_4\mfe_structure_' d '.txt'];
[mfes,anti_inds,bulges1,bulges2,endbulges,seq_id]= ...

```

```

    read_structure_from_mfe(palmfefile);
palbpfile = ['c:\rosetta\data_baseline_13_4\bp_prob_' d '.txt'];
[bp_probs,len] = read_bp(palbpfile);
if randomize
    rand('state',sum(100*clock));
    disp('performing randomized permutation');
    l = randperm(length(seqs));
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    endbulges = endbulges(l);
    pallen = pallen(l);
    mirlen = mirlen(l);
    pos = pos(l);
    seq_id = seq_id(l);
    seqs = seqs(l);
    mirseqs = mirseqs(l);
    mfes = mfes(l);
    bp_probs = bp_probs(l);
    anti_inds = anti_inds(l);
end
if remove_duplicate_mirs
    disp('removing duplicate mirs');
    D = zeros(length(seqs),1); % list of duplicate mirs
    for i = 1:length(seqs)
        for j = i+1:length(seqs)
            if length(mirseqs{j}) == length(mirseqs{i})
                if all(mirseqs{j} == mirseqs{i})
                    D(j) = 1;
                    break;
                end
            end
        end
    end
    l = find(D);
    bulges1(l) = [];
    bulges2(l) = [];
    endbulges(l) = [];
    mirlen(l) = [];
    pallen(l) = [];
    pos(l) = [];
    seq_id(l) = [];
    seqs(l) = [];
    mirseqs(l) = [];
    mfes(l) = [];
    bp_probs(l) = [];
    anti_inds(l) = [];
end
data_dir = 'data_baseline_29_7';
if(~exist('set_name'))
    set_name = 'h156';

```

```

end
if ~exist('randomize')
    randomize = 0;
end
if ~exist('remove_duplicate_mirs')
    remove_duplicate_mirs = 0;
end
palfile = ['c:\rosetta\' data_dir \'zucker_draw_' set_name '.txt'];
fid = fopen(palfile,'r');
[seqs,anti_inds,bulges1,bulges2,endbulges,pal_ids,energy,all_pal_ids] = ...
    read_structure_with_id_fid(fid,10000000000);
fclose(fid);
mirseqfile = ['c:\rosetta\' data_dir \'mirseq_' set_name '.txt'];
[mirseqs,mirlen,mir_ids,all_mir_ids] = read_seq_with_id(mirseqfile);
if(length(all_mir_ids)~=length(all_pal_ids) | any(all_mir_ids-all_pal_ids))
    error('ids in palfile and mirfile must match and be in same order');
end
if(length(mir_ids)~=length(pal_ids) | any(mir_ids-pal_ids))
    error('in one of the files (mir or pal) there was an illegal sequence not illegal in other file');
end
pos = locate_dicer(mirseqs,seqs);
if randomize
    rand('state',sum(100*clock));
    disp('performing randomized permutation');
    l = randperm(length(seqs));
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    anti_inds = anti_inds(l);
    endbulges = endbulges(l);
    mirlen = mirlen(l);
    pos = pos(l);
    pal_ids = pal_ids(l);
    seqs = seqs(l);
    mirseqs = mirseqs(l);
    mir_ids = mir_ids(l);
end
if remove_duplicate_mirs
    disp('removing duplicate mirs');
    D = zeros(length(seqs),1); % list of duplicate mirs
    for i = 1:length(seqs)
        for j = i+1:length(seqs)
            if length(mirseqs{j}) == length(mirseqs{i})
                if all(mirseqs{j} == mirseqs{i})
                    D(j) = 1;
                    break;
                end
            end
        end
    end
    I = find(D);
end

```

```

bulges1(l) = [];
bulges2(l) = [];
anti_inds(l) = [];
endbulges(l) = [];
mirlen(l) = [];
pos(l) = [];
pal_ids(l) = [];
seqs(l) = [];
mirseqs(l) = [];
mir_ids(l) = [];
end
lend=mirlen; % some applications use lend and not mirlen.
function pos = locate_dicer(dicer_seq,pal_seq);
%pos = locate_dicer(dicer_seq,palseq)
%get absolute position of dicer on palindrom, from the beginning of the palindrom
if length(dicer_seq) ~= length(pal_seq)
    error('different number of sequences');
end
%convert to nucleotide-format if in int format
if all(~isletter(pal_seq{1}))
    for i = 1:length(pal_seq)
        pal_seq{i} = int2nuc(pal_seq{i},'uppercase');
    end
end
if all(~isletter(dicer_seq{1}))
    for i = 1:length(dicer_seq)
        dicer_seq{i} = int2nuc(dicer_seq{i},'uppercase');
    end
end
pos = zeros(1,length(dicer_seq));
for i = 1:length(dicer_seq)
    l = findstr(dicer_seq{i}, pal_seq{i});
    if length(l) == 1
        pos(i) = l;
    else
        pos(i) = NaN;
    end
end
function y = meannan(x)
if(min(size(x))==1)
    y = mean(x(~isnan(x)));
    return;
end
y = zeros(1,size(x,2));
for i=1:size(x,2)
    v = x(:,i);
    y(i) = mean(v(~isnan(v)));
end
function seqsbp = nuc2bp(seqs,anti_inds,base_pair_basis)
%seqsbp = nuc2bp(seqs,anti_inds,base_pair_basis)

```

```

%transform to base pair representation
%for a 3 state model {AT,CG,TG} -> 1 2 3
%for a 6 state {AT,CG,TG,TA,GC,GT} -> 1 2 3 4 5 6
%also works if seqs is a vector and not a cell array, in which case returns a vector
if(~iscell(seqs))
    tt{1} = seqs;
    seqs = tt;
    tt{1} = anti_inds;
    anti_inds = tt;
    vecflag = 1;
else
    vecflag = 0;
end
map = zeros(4);
map(1,3) = 1; %AT
map(2,4) = 2; %CG
map(3,4) = 3; %TG
if base_pair_basis == 3
    map = map+map';
else
    map(3,1) = 4; %AT
    map(4,2) = 5; %CG
    map(4,3) = 6; %TG
end
seqsbp = cell(size(seqs));
for i = 1:length(seqs)
    seqsi = seqs{i};
    seqsbpi = zeros(size(seqsi));
    anti_indsi = anti_inds{i};

    I = find(anti_indsi ~= 0);
    for j = 1:length(I)
        ij = I(j);
        seqsbpi(ij) = map(seqsi(ij),seqsi(anti_indsi(ij)));
    end
    seqsbp{i} = seqsbpi;
end
if(vecflag)
    tt=seqsbp{1};
    seqsbp = tt;
end
return
function [intseq, fault_seq] = nuc2int(strseq);
%[intseq, fault_seq] = nuc2int(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
if(~isletter(strseq(1)))
    intseq = strseq;
    fault_seq = 0;
    return;
end

```



```

intseq = zeros(size(strseq));
fault_seq = 0;
for i = 1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i) = 1;
        case 'C' , intseq(i) = 2;
        case 'T' , intseq(i) = 3;
        case 'G' , intseq(i) = 4;
        otherwise , intseq = []; fault_seq = 1; break;
    end
end
function intseq = nuc2int4(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
strseq = deblank(strseq);
intseq = zeros(size(strseq));
for i = 1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i) = 1;
        case 'C' , intseq(i) = 2;
        case 'T' , intseq(i) = 3;
        case 'G' , intseq(i) = 4;
        otherwise , intseq(i) = [];
    end
end
function [intseq, fault_seq] = nuc2int4_new(strseq);
%[intseq, fault_seq] = nuc2int4_new(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
intseq = zeros(size(strseq));
fault_seq = 0;
for i = 1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i) = 1;
        case 'C' , intseq(i) = 2;
        case 'T' , intseq(i) = 3;
        case 'G' , intseq(i) = 4;
        otherwise , intseq = []; fault_seq = 1; break;
    end
end
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);

```

```

bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
next_pal_id = str2double(fgetl(fid));
while ~feof(fid) & seq_no < seqtot
    this_pal_id = next_pal_id;
    this_energy = str2double(fgetl(fid));
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    fault_seq_emptyline = 0;
    while((line~-1 & isnan(str2double(line))) | isempty(line))
        if(isempty(line))
            fault_seq_emptyline = 1;
        end
        i = i+1;
        structure(i,1:length(line)) = line;
        line = fgetl(fid);
    end
    if(~feof(fid))
        next_pal_id = str2double(line);
    end
    if(i~=4)
        fault_seq_numlines = 1;
    else
        fault_seq_numlines = 0;
    end

    fault_seq_struct = 1; % guilty until proven innocent
    fault_seq_nuc = 1;
    if(fault_seq_numlines == 0 & fault_seq_emptyline==0)
        [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
        if(fault_seq_struct==0)
            % this is the old bulge1 and bulge2, now need to correct that
            bulge_nonsymi=bulge1i;
            bulge_symi=bulge2i;
            for j = 1:length(seqi)
                if(bulge_nonsymi(j))
                    if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                        bulge_symi(j) = 1;
                        bulge_nonsymi(j) = 0;
                    end
                end
            end
            for j = length(seqi):-1:1
                if(bulge_nonsymi(j))
                    if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                        bulge_symi(j) = 1;

```

```

        bulge_nonsymi(j) = 0;
    end
end
end
end
[intseq, fault_seq_nuc] = nuc2int4_new(seqi);
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    if(fault_seq_emptyline)
        disp(['reason is that there was an empty line in zucker']);
    elseif(fault_seq_numlines)
        disp(['reason is that there were not 4 lines in the draw']);
    elseif(fault_seq_struct)
        disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
    elseif(fault_seq_nuc)
        disp(['reason is that there was an illegal letter in the seq']);
    end
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col = 1: max_col
    fl = find(isletter(uphalf(:,col)));

```

```

if (length(fl)>1);
    fault_seq = 1;
    seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
    return;
end;
if ~isempty(fl)
    count = count + 1;
    seq(count) = uphalf(fl,col);
    bulge = (fl == bulge_row);
    if(bulge)
        tmpmat(1,col) = 0;
    else
        tmpmat(1,col) = count;
    end
    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
    end
end

```

```

    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
    endbulge(count) = 0;
end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
% in this check_e version returns faulty seq also when no energy found
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
next_pal_id = str2double(fgetl(fid));
while ~feof(fid) & seq_no < seqtot
    this_pal_id = next_pal_id;
    this_energy = str2double(fgetl(fid));
    if(isnan(this_energy))
        fault_seq_energy = 1;
    else
        fault_seq_energy = 0;
    end
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    fault_seq_emptyline = 0;
    while((line~-1 & isnan(str2double(line))) | isempty(line))
        if(isempty(line))

```

```

        fault_seq_emptyline = 1;
    end
    i = i+1;
    structure(i,1:length(line)) = line;
    line = fgetl(fid);
end
if(~feof(fid))
    next_pal_id = str2double(line);
end
if(i~=4)
    fault_seq_numlines = 1;
else
    fault_seq_numlines = 0;
end

fault_seq_struct = 1; % guilty until proven innocent
fault_seq_nuc = 1;
if(fault_seq_numlines == 0 & fault_seq_emptyline==0 & fault_seq_energy==0)
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
    if(fault_seq_struct==0)
        % this is the old bulge1 and bulge2, now need to correct that
        bulge_nonsymi=bulge1i;
        bulge_symi=bulge2i;
        for j = 1:length(seqi)
            if(bulge_nonsymi(j))
                if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        for j = length(seqi):-1:1
            if(bulge_nonsymi(j))
                if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
    end
    [intseq, fault_seq_nuc] = nuc2int4_new(seqi);
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0 &
fault_seq_energy==0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
end

```

```

endbulges{seq_no} = endbulgei;
pal_id(seq_no) = this_pal_id;
energy(seq_no) = this_energy;
counter = counter + 1;
all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    if(fault_seq_energy)
        disp(['reason is that there was no energy']);
    elseif(fault_seq_emptyline)
        disp(['reason is that there was an empty line in zucker']);
    elseif(fault_seq_numlines)
        disp(['reason is that there were not 4 lines in the draw']);
    elseif(fault_seq_struct)
        disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
    elseif(fault_seq_nuc)
        disp(['reason is that there was an illegal letter in the seq']);
    end
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col = 1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1);
        fault_seq = 1;
        seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
        return;
    end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else

```

```

        tmpmat(1,col) = count;
    end
    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))

```



```

    anti_ind(tmpmat(1,col)) = tmpmat(2,col);
    anti_ind(tmpmat(2,col)) = tmpmat(1,col);
end
end
return
function [xp2,yp2] = plot_errors_bins2(pos_error,score,N)
% measure the distribution of erros
if length(pos_error) ~= length(score)
    error('pos_estimated and score not compatible');
end
if ~exist('N')
    N = 6;
end
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
dist1 = zeros(0); %correct size, distance = 1;
dist2 = zeros(0);
dith = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos_error);
for i = 1:length(thresh)-1
    I = find(score <= thresh(i) & score >= thresh(i+1));
    if ~isempty(I)
        count = count + 1;
        midbin(count) = mean(score(I));

        accuracy(count) = sum(pos_error(I) == 0)/length(I);
        J1 = find(abs(pos_error(I)) == 1);
        dist1(count) = length(J1)/length(I);
        J2 = find(abs(pos_error(I)) == 2);
        dist2(count) = length(J2)/length(I);
        Jh = find(abs(pos_error(I)) > 2);
        dith(count) = length(Jh)/length(I);
        fraction(count) = length(I)/N;
    else
        count = count+1;
        midbin(count) = NaN;;
        accuracy(count) = NaN;
        dist1(count) = NaN;
        dist2(count) = NaN;
        dith(count) = NaN;
        fraction(count) = NaN;
    end
end
acc1 = accuracy + dist1;
acc2 = accuracy + dist1 + dist2;
hold on
plot(midbin, acc2,'g')

```

```

plot(midbin, acc1,'r')
plot(midbin, accuracy,'b')
plot(midbin,fraction,'c')
legend('dist \leq 2', 'dist \leq 1', 'precise',2);
plot(midbin, acc2,'*g')
plot(midbin, acc1,'or')
plot(midbin, accuracy,'bd')
xlabel('bin');
%axis([min(midbin)-1 max(midbin)+1 0 1])
[ry,yp2,mass,xp2,newy,pos] = isotonic_regression(midbin,acc2);
yp2(end)
returnfunction plot_errors_perc(pos_error,score)
% measure the distribution of erros
N = 100;
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
dist1 = zeros(0); %correct size, distance = 1;
dist2 = zeros(0);
dith = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos_error);
for i = 1:length(thresh)
    I = find(score >= thresh(i));
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_error(I) == 0)/length(I);
        J1 = find(abs(pos_error(I)) == 1);
        dist1(count) = length(J1)/length(I);
        J2 = find(abs(pos_error(I)) == 2);
        dist2(count) = length(J2)/length(I);
        Jh = find(abs(pos_error(I)) > 2);
        dith(count) = length(Jh)/length(I);
        fraction(count) = length(I)/N;
    else
        count = count+1;
        accuracy(count) = NaN;
        dist1(count) = NaN;
        dist2(count) = NaN;
        dith(count) = NaN;
        fraction(count) = NaN;
    end
end

acc1 = accuracy + dist1;
acc2 = accuracy + dist1 + dist2;
%clf
hold on

```

```

plot(perc, acc2,'g')
plot(perc, acc1,'r')
plot(perc, accuracy,'b')
plot(perc, thresh,'c')
legend('dist \leq 2', 'dist \leq 1', 'precise', 'threshold',2);
xlabel('percentage');
axis([0 100 0 1]);

%keyboard
%prepare result
N = length(accuracy);
res = [accuracy(N), acc1(N), acc2(N), acc2(round(0.2*N))]
returnfunction y = prctile(x,p);
%PRCTILE gives the percentiles of the sample in X.
% Y = PRCTILE(X,P) returns a value that is greater than P percent
% of the values in X. For example, if P = 50 Y is the median of X.
%
% P may be either a scalar or a vector. For scalar P, Y is a row
% vector containing Pth percentile of each column of X. For vector P,
% the ith row of Y is the P(i) percentile of each column of X.
% Copyright (c) 1993-98 by The MathWorks, Inc.
% $Revision: 2.6 $ $Date: 1997/11/29 01:46:27 $
[prows pcols] = size(p);
if prows ~= 1 & pcols ~= 1
    error('P must be a scalar or a vector.');
```

```

end
if any(p > 100) | any(p < 0)
    error('P must take values between 0 and 100');
```

```

end
xx = sort(x);
[m,n] = size(x);
if m==1 | n==1
    m = max(m,n);
    if m == 1,
        y = x*ones(length(p),1);
        return;
    end
    n = 1;
    q = 100*(0.5:m - 0.5)./m;
    xx = [min(x); xx(:); max(x)];
else
    q = 100*(0.5:m - 0.5)./m;
    xx = [min(x); xx; max(x)];
end
q = [0 q 100];
y = interp1(q,xx,p);
function [bps,len] = read_bp(filename);
%[bps,len] = read_bp(filename);
%reads bp file into cell array. bps{i} is a 3col matrix of the bp probs
%len(i) is the length of the ith palindrom (appears as info in the bp file)

```

```

fid = fopen(filename,'r');
if fid == -1
    error([' file ' filename ' could not be opened']);
end
seq_no = 0;
while ~feof(fid)
    pallen = str2num(fgetl(fid));
    arm5 = str2num(fgetl(fid));
    arm3 = str2num(fgetl(fid));
    p = str2num(fgetl(fid));
    seq_no = seq_no+1;
    bps{seq_no} = [arm5',arm3',p'];
    len(seq_no) = pallen;
end
fclose(fid);
return

```

```

function [seqs,len] = read_seq(filename);
%[seqs,len] = read_seq(filename);
%reads dicer or pal sequences into cell array, in numeric format
fid = fopen(filename,'r');
if fid == -1
    error([' file ' filename ' could not be opened']);
end
id = 0;
seq_no = 0;
while ~feof(fid)
    line = fgetl(fid);
    line = deblank(line);
    [intseq, fault_seq] = nuc2int4_new(line);
    id = id + 1;
    if fault_seq == 0
        seq_no = seq_no + 1;
        seqs{seq_no} = intseq;
        len(seq_no) = length(intseq);
    else
        disp(['faulty seq on id ' num2str(id)])
    end

    if(mod(seq_no,1000) == 0 & seq_no ~= 0)
        disp(['seq_no ' num2str(seq_no)]);
    end
end
fclose(fid);
return

```

```

function [seqs,len, ids,all_ids] = read_seq_with_id(filename);
%[seqs,len,ids,all_ids] = read_seq_id(filename);
%reads mirr or pal sequences into cell array, in numeric format
%the input file must contain for each seq 2 lines, first is id, second is the seq

```

% ids holds the ids of those that were read successfully so has same length as seqs

% all_ids is all ids encountered in the file regardless of whether were legal

```
fid = fopen(filename,'r');
```

```
if fid == -1
```

```
    error(['file ' filename ' could not be opened']);
```

```
end
```

```
id = 0;
```

```
seq_no = 0;
```

```
all_ids = [];
```

```
while ~feof(fid)
```

```
    this_id = str2num(fgetl(fid));
```

```
    all_ids = [all_ids,this_id];
```

```
    line = fgetl(fid);
```

```
    line = deblank(line);
```

```
    [intseq, fault_seq] = nuc2int4_new(line);
```

```
    if fault_seq == 0
```

```
        seq_no = seq_no + 1;
```

```
        seqs{seq_no} = intseq;
```

```
        len(seq_no) = length(intseq);
```

```
        ids(seq_no) = this_id;
```

```
    else
```

```
        disp(['faulty seq on id ' num2str(id)])
```

```
    end
```

```
if(mod(seq_no,1000) == 0 & seq_no ~= 0)
```

```
    disp(['seq_no ' num2str(seq_no)]);
```

```
end
```

```
end
```

```
fclose(fid);
```

```
return
```

```
function [mfes,anti_inds,bulges_nonsym,bulges_sym,endbulges,seq_id]= read_structure_from_mfe(filename);
```

```
% read rnafold structure
```

```
% seq is a cell array containing sequences (in ints)
```

```
% anti_inds holds for each nuc in the seq what is the index of the nuc across from it where the 0 means unpaired.
```

```
% bulge_nonsym is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
```

```
% bulge_sym is similarly for 2 sided bulge
```

```
% note that any nuc in a bulge which has a bulge across gets bulge_sym even if it itself is across a -
```

```
% this is the difference from the original read_structure
```

```
% endbulge is a cell array with binary strings with 1 on the end bulge only
```

```
% the input file contains 3 lines for each palindrom. the first line is a single number indicating the pal length
```

```
% the second and third lines are the base pairs in the mfe structure
```

```
fid = fopen(filename,'r');
```

```
seq_no = 0;
```

```
mfe = cell(0);
```

```
bulges_nonsym= cell(0);
```

```
bulges_sym= cell(0);
```

```
endbulges = cell(0);
```

```
while ~feof(fid)
```

```

pallen = str2num(fgetl(fid));
arm5 = str2num(fgetl(fid));
arm3 = str2num(fgetl(fid));
seq_no = seq_no+1;

mfes{seq_no} = [arm5',arm3'];

ai = zeros(1,pallen);
ai(arm5) = arm3;
ai(arm3) = arm5;
anti_inds{seq_no} = ai;

ebs = zeros(1,pallen);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
ebs(eb_start:eb_end) = 1;
endbulges{seq_no} = ebs;
if(eb_end-eb_start+1 < 3)
    disp(['end bulge shorter than 3 nucs in seq no ' num2str(seq_no)]);
end

bs = zeros(1,pallen);
bns = zeros(1,pallen);
arm5t = [0,arm5];
arm3t = [pallen+1,arm3];
for i=2:length(arm5t)
    d5 = arm5t(i)-arm5t(i-1)-1;
    d3 = arm3t(i-1)-arm3t(i)-1;
    if(d5)
        if(d3)
            bs([arm5t(i-1)+1:arm5t(i)-1 , arm3t(i)+1:arm3t(i-1)-1])=1;
        else
            bns(arm5t(i-1)+1:arm5t(i)-1) = 1;
        end
    else
        if(d3)
            bns(arm3t(i)+1:arm3t(i-1)-1) = 1;
        end
    end
end
bulges_sym{seq_no} = bs;
bulges_nonsym{seq_no} = bns;

end
seq_id = 1:seq_no;
fclose(fid);

function [seqs,bulges_nonsym,bulges_sym,endbulges,seq_id] = read_structure_new(filename);
% read zucker structure
% seq is a cell array containing sequences

```

```

% bulge_nonsym is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
% bulge_sym is similarly for 2 sided bulge
% note that any nuc ina bulge which has a bulge across gets bulge_sym even if it itself is across a -
% this is the difference from the original read_structure
% endbulge is a cell array with binary strings with 1 on the end bulge only
Mxplen = 250; % maximal length of palindrom
fid = fopen(filename,'r');
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
seq_id = zeros(0);
id = 0;
while ~feof(fid)
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    id = id +1;
    [seqi, bulge1i, bulge2i, endbulgei] = get_features(structure);
    % this is the old bulge1 and bulge2, now need to correct that
    bulge_nonsymi=bulge1i;
    bulge_symi=bulge2i;
    for j = 1:length(seqi)
        if(bulge_nonsymi(j))
            if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                bulge_symi(j) = 1;
                bulge_nonsymi(j) = 0;
            end
        end
    end
end
for j = length(seqi):-1:1
    if(bulge_nonsymi(j))
        if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
            bulge_symi(j) = 1;
            bulge_nonsymi(j) = 0;
        end
    end
end
end

[intseq, fault_seq] = nuc2int4_new(seqi);
if fault_seq == 0
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    seq_id(seq_no) = id;
end

```

```

else
    disp(['faulty seq on id ' num2str(id)])
end
if(mod(seq_no,1000) == 0)
    seq_no
end
end
fclose(fid);
return
function [seq, bulge1, bulge2, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));

```



```

if ~isempty(fl)
    count = count + 1;
    seq(count) = lwhalf(fl,col);
    bulge = (fl == bulge_row);
    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
    endbulge(count) = 0;
end
end
return

```

```

function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
while ~feof(fid) & seq_no < seqtot
    this_pal_id = str2double(fgetl(fid));
    this_energy = str2double(fgetl(fid));
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    if(isempty(line))
        line = 'emptyline';
        fault_seq_emptyline = 1;
    else
        fault_seq_emptyline = 0;
    end
    while(line(1)~= '|') % if emptyline this is always true so will go into loop
        i = i+1;
        structure(i,1:length(line)) = line;
        line = fgetl(fid);
        if(isempty(line))

```

```

        line = 'emptyline';
        fault_seq_emptyline = 1;
    end
end
if(i~=4)
    fault_seq_numlines = 1;
else
    fault_seq_numlines = 0;
end

fault_seq_struct = 1; % guilty until proven innocent
fault_seq_nuc = 1;
if(fault_seq_numlines == 0 & fault_seq_emptyline==0)
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
    if(fault_seq_struct==0)
        % this is the old bulge1 and bulge2, now need to correct that
        bulge_nonsymi=bulge1i;
        bulge_symi=bulge2i;
        for j = 1:length(seqi)
            if(bulge_nonsymi(j))
                if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        for j = length(seqi):-1:1
            if(bulge_nonsymi(j))
                if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        [intseq, fault_seq_nuc] = nuc2int4_new(seqi);
    end
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else

```

```

disp(['faulty seq on pal id ' num2str(this_pal_id)])
if(fault_seq_emptyline)
    disp(['reason is that there was an empty line in zucker']);
elseif(fault_seq_numlines)
    disp(['reason is that there were not 4 lines in the draw']);
elseif(fault_seq_struct)
    disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
elseif(fault_seq_nuc)
    disp(['reason is that there was an illegal letter in the seq']);
end
counter = counter + 1;
all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1);
        fault_seq = 1;
        seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
        return;
    end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end

```

```

        end
    end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col = max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)

```

```

% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
% in this check_e version returns faulty seq also when no energy found
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
while ~feof(fid) & seq_no < seqtot
    this_pal_id = str2double(fgetl(fid));
    this_energy = str2double(fgetl(fid));
    if(isnan(this_energy))
        fault_seq_energy = 1;
    else
        fault_seq_energy = 0;
    end
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    if isempty(line)
        line = 'emptyline';
        fault_seq_emptyline = 1;
    else
        fault_seq_emptyline = 0;
    end
    while(line(1)~= '|') % if emptyline this is always true so will go into loop
        i = i+1;
        structure(i,1:length(line)) = line;
        line = fgetl(fid);
        if isempty(line)
            line = 'emptyline';
            fault_seq_emptyline = 1;
        end
    end
end
if(i~=4)
    fault_seq_numlines = 1;
else
    fault_seq_numlines = 0;
end

fault_seq_struct = 1; % guilty until proven innocent
fault_seq_nuc = 1;
if(fault_seq_numlines == 0 & fault_seq_emptyline==0 & fault_seq_energy==0)
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);

```

```

if(fault_seq_struct==0)
    % this is the old bulge1 and bulge2, now need to correct that
    bulge_nonsymi=bulge1i;
    bulge_symi=bulge2i;
    for j = 1:length(seqi)
        if(bulge_nonsymi(j))
            if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                bulge_symi(j) = 1;
                bulge_nonsymi(j) = 0;
            end
        end
    end
    for j = length(seqi):-1:1
        if(bulge_nonsymi(j))
            if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                bulge_symi(j) = 1;
                bulge_nonsymi(j) = 0;
            end
        end
    end
    [intseq, fault_seq_nuc] = nuc2int4_new(seqi);
end
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0 &
fault_seq_energy==0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    if(fault_seq_energy)
        disp(['reason is that there was no energy']);
    elseif(fault_seq_emptyline)
        disp(['reason is that there was an empty line in zuker']);
    elseif(fault_seq_numlines)
        disp(['reason is that there were not 4 lines in the draw']);
    elseif(fault_seq_struct)
        disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
    elseif(fault_seq_nuc)
        disp(['reason is that there was an illegal letter in the seq']);
    end
    counter = counter + 1;
end

```

```

    all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col = 1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1);
        fault_seq = 1;
        seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
        return;
    end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
end

```

```

    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col = max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);

```



```

pal_id = zeros(0);
energy = zeros(0);
while ~feof(fid) & seq_no < seqtot
    this_pal_id = str2num(fgetl(fid));
    this_energy = str2num(fgetl(fid));
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei] = get_features(structure);
    % this is the old bulge1 and bulge2, now need to correct that
    bulge_nonsymi=bulge1i;
    bulge_symi=bulge2i;
    for j = 1:length(seqi)
        if(bulge_nonsymi(j))
            if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                bulge_symi(j) = 1;
                bulge_nonsymi(j) = 0;
            end
        end
    end
end
for j = length(seqi):-1:1
    if(bulge_nonsymi(j))
        if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
            bulge_symi(j) = 1;
            bulge_nonsymi(j) = 0;
        end
    end
end
end

[intseq, fault_seq] = nuc2int4_new(seqi);
if fault_seq == 0
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
end
end
end
return

```

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1); keyboard;end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards form 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));

```

```

if ~isempty(fl)
    count = count + 1;
    seq(count) = lwhalf(fl,col);
    bulge = (fl == bulge_row);
    if(bulge)
        tmpmat(2,col) = 0;
    else
        tmpmat(2,col) = count;
    end
    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
    endbulge(count) = 0;
end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,seq_id] = read_structure_withanti(filename);
% read zucker structure
% seq is a cell array containing sequences (in ints)
% anti_inds holds for each nuc in the seq what is the index of the nuc across from it where the 0 means unpaired.
% bulge_nonsym is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
% bulge_sym is similarly for 2 sided bulge
% note that any nuc in a bulge which has a bulge across gets bulge_sym even if it itself is across a -
% this is the difference from the original read_structure
% endbulge is a cell array with binary strings with 1 on the end bulge only
Mxplen = 250; % maximal length of palindrom
fid = fopen(filename,'r');
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
seq_id = zeros(0);
id = 0;
while ~feof(fid)
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
end

```

```

end
id = id + 1;
[seqi, anti_indi, bulge1i, bulge2i, endbulgei] = get_features(structure);
% this is the old bulge1 and bulge2, now need to correct that
bulge_nonsymi=bulge1i;
bulge_symi=bulge2i;
for j = 1:length(seqi)
    if(bulge_nonsymi(j))
        if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
            bulge_symi(j) = 1;
            bulge_nonsymi(j) = 0;
        end
    end
end
for j = length(seqi):-1:1
    if(bulge_nonsymi(j))
        if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
            bulge_symi(j) = 1;
            bulge_nonsymi(j) = 0;
        end
    end
end

[intseq, fault_seq] = nuc2int4_new(seqi);
if fault_seq == 0
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    seq_id(seq_no) = id;
else
    disp(['faulty seq on id ' num2str(id)])
end
if(mod(seq_no,1000) == 0)
    seq_no
end
end
fclose(fid);
return
function [seq, anti_ind, bulge1, bulge2, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);

```

```

count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1); keyboard;end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards form 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
    end
end

```

```

    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
    endbulge(count) = 0;
end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
end

return

```

```

function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,seq_id] = read_structure_withanti_fid(fid,seqtot);
%[seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,seq_id] = read_structure_withanti_fid(fid,seqtot);
% read zucker structure
% seq is a cell array containing sequences (in ints)
% anti_inds holds for each nuc in the seq what is the index of the nuc across from it where the 0 means unpaired.
% bulge_nonsym is a cell array with binary strings with 1 for one sided bulge (not incl. end bulge)
% bulge_sym is similarly for 2 sided bulge
% note that any nuc in a bulge which has a bulge across gets bulge_sym even if it itself is across a -
% this is the difference from the original read_structure
% endbulge is a cell array with binary strings with 1 on the end bulge only
Mxplen = 250; % maximal length of palindrom
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
seq_id = zeros(0);
id = 0;
while ~feof(fid) & seq_no < seqtot
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    id = id +1;
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei] = get_features(structure);
    % this is the old bulge1 and bulge2, now need to correct that
    bulge_nonsymi=bulge1i;
    bulge_symi=bulge2i;
    for j = 1:length(seqi)
        if(bulge_nonsymi(j))
            if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on

```

```

        bulge_symi(j) = 1;
        bulge_nonsymi(j) = 0;
    end
end
end
for j = length(seqi):-1:1
    if(bulge_nonsymi(j))
        if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
            bulge_symi(j) = 1;
            bulge_nonsymi(j) = 0;
        end
    end
end
end

[intseq, fault_seq] = nuc2int4_new(seqi);
if fault_seq == 0
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    seq_id(seq_no) = id;
else
    disp(['faulty seq on id ' num2str(id)])
end
end
return
function [seq, anti_ind, bulge1, bulge2, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1); keyboard;end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
    end
end

```

```

    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
end
end
% endbulge is coded on the upper half
% go backwards form 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end

```



```

end
end

```

```

return

```

```

function y = stdnan(x)
if(min(size(x))==1)
    y = std(x(~isnan(x)));
    return;
end

```

```

y = zeros(1,size(x,2));
for i=1:size(x,2)
    v = x(:,i);
    y(i) = std(v(~isnan(v)));
end

```

```

function [sym_in_win, sym_out, faulty] = symm(pal_len,mfe,winstart5,win_len)
% function [sym_in_win, sym_out, faulty] = symm(pal_len, mfe,winstart5,win_len)
% if window is illegal, returns faulty=1 and NAN for other values
% pal_len is length of palindrom
% mfe has the pairs in the min free energy drawing
% winstart5 is the positon of the start of the window in question
% win_len is its length
% sym_in_win = number of unpaired bases in win - number in antiwin, normalized by their sum
% if win start/ends within a bulge takes in anti a proportional number of bases
% sym_out is number of unpaired on window arm - opposite arm - sym_in_win, normalized by
% total number of unpaired in both arms - those unpaired in win
% NOTE that both have a sign defined by the arm onwhich the window sits.
% also note that no check is made on winstart5 and win_len being positive (which they must) - beware!

```

```

arm5 = mfe(:,1);
arm3 = mfe(:,2);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1; % num nucs in end bulge
win_end = winstart5+win_len-1;
win_inds = [winstart5:win_end];
if(any(intersect(win_inds,[eb_start:eb_end])) | win_end>pal_len)
    faulty =1;
    sym_in_win = NaN;
    sym_out = NaN;
    disp('WINDOW IS ILLEGAL. RETURNING FAULTY=1. ');
    disp(['window has ' num2str(length(intersect(win_inds,[eb_start:eb_end]))) ' nucs in endloop']);
    return
end

```

```

faulty = 0;
m5 = diff(arm5)-1;
m3 = -1*diff(arm3)-1;
d53 = m5-m3;
if(winstart5<eb_start)
    win_arm5 = 1; % win on arm5
end

```

```

else
    win_arm5 = 0;
end
% create the vector bulges from the mfe structure!
bulges = ones(1,pal_len);
bulges(arm5) = 0;
bulges(arm3) = 0;
bulged5 = sum(bulges(1:eb_start-1));
bulged3 = sum(bulges(eb_end+1:end));
bulges_win = bulges(win_inds);
inwin = sum(bulges_win);
% sum antiwin without bulges
if(win_arm5)
    tt=find(arm5-winstart5 >= 0);
    ind1=tt(1); % index in arm5 of first base in win that is paired
    antiend = arm3(ind1);
    tt=find(arm5-win_end <= 0);
    ind2=tt(end); % as ind1 but last
    antistart = arm3(ind2);
    inantiwin = sum(bulges(antistart:antiend)); % without bulges at ends of anti
    if(bulges_win(1))
        if(ind1>1)
            partonwin = (arm5(ind1)-winstart5)/(arm5(ind1)-arm5(ind1-1)-1);
            inantiwin = inantiwin + (arm3(ind1-1)-arm3(ind1)-1)*partonwin;
        else
            partonwin = (arm5(ind1)-winstart5)/(arm5(ind1)-1);
            inantiwin = inantiwin + (length(bulges)-arm3(ind1))*partonwin;
        end
    end
end
if(bulges_win(end))
    partonwin = (win_end-arm5(ind2))/(arm5(ind2+1)-arm5(ind2)-1);
    inantiwin = inantiwin + (arm3(ind2)-arm3(ind2+1)-1)*partonwin;
end
dd = inwin-inantiwin;
sdd = inwin+inantiwin;
if(sdd)
    sym_in_win = dd / sdd;
else % dd must also be 0
    sym_in_win = 0;
end
if(bulged5+bulged3-sdd)
    sym_out = (bulged5-bulged3-dd) / (bulged5+bulged3-sdd);
else
    sym_out = 0;
end
else
    tt=find(arm3-winstart5 >= 0);
    ind1=tt(end); % index in arm3 of first base in win that is paired
    antiend = arm5(ind1);
    tt=find(arm3-win_end <= 0);

```

```

ind2=tt(1); % index in arm3 of last base in win that is paired
antistart = arm5(ind2);
inantiwin = sum(bulges(antistart:antiend)); % without bulges at ends of anti
if(bulges_win(1))
    partonwin = (arm3(ind1)-winstart5)/(arm3(ind1)-arm3(ind1+1)-1);
    inantiwin = inantiwin + (arm5(ind1+1)-arm5(ind1)-1)*partonwin;
end
if(bulges_win(end))
    if(ind2>1)
        partonwin = (win_end-arm3(ind2))/(arm3(ind2-1)-arm3(ind2)-1);
        inantiwin = inantiwin + (arm5(ind2)-arm5(ind2-1)-1)*partonwin;
    else
        partonwin = (win_end-arm3(ind2))/(length(bulges)-arm3(ind2));
        inantiwin = inantiwin + (arm5(ind2)-1)*partonwin;
    end
end
dd = inwin-inantiwin;
sdd = inwin+inantiwin;
if(sdd)
    sym_in_win = dd / sdd;
else % dd must also be 0
    sym_in_win = 0;
end
if(bulged3+bulged5-sdd)
    sym_out = (bulged3-bulged5-dd) / (bulged3+bulged5-sdd);
else
    sym_out = 0;
end
end
function [sym_in_win, sym_out, faulty] = symm2(pal_len,mfe,winstart5,win_len)
% function [sym_in_win, sym_out, faulty] = symm2(pal_len, mfe,winstart5,win_len)
% like symm but no normalization
arm5 = mfe(:,1);
arm3 = mfe(:,2);
eb_start = arm5(end)+1;
eb_end = arm3(end)-1;
eb_len = eb_end-eb_start+1; % num nucs in end bulge
win_end = winstart5+win_len-1;
win_inds = [winstart5:win_end];
if(any(intersect(win_inds,[eb_start:eb_end])) | win_end>pal_len)
    faulty =1;
    sym_in_win = NaN;
    sym_out = NaN;
    disp('WINDOW IS ILLEGAL. RETURNING FAULTY=1. ');
    disp(['window has ' num2str(length(intersect(win_inds,[eb_start:eb_end]))) ' nucs in endloop']);
    return
end
faulty = 0;
win_arm5 =(winstart5<eb_start);
% create the vector bulges from the mfe structure!

```

```

bulges = ones(1,pal_len);
bulges(arm5) = 0;
bulges(arm3) = 0;
bulges(eb_start:eb_end) = 0;
bulged5 = sum(bulges(1:eb_start-1));
bulged3 = sum(bulges(eb_end+1:end));
bulges_win = bulges(win_inds);
inwin = sum(bulges_win);
% sum antiwin without bulges
if(win_arm5)
    tt=find(arm5-winstart5 >= 0);
    ind1=tt(1); % index in arm5 of first base in win that is paired
    antiend = arm3(ind1);
    tt=find(arm5-win_end <= 0);
    ind2=tt(end); % as ind1 but last
    antistart = arm3(ind2);
    inantiwin = sum(bulges(antistart:antiend)); % without bulges at ends of anti
    if(bulges_win(1))
        if(ind1>1)
            partonwin = (arm5(ind1)-winstart5)/(arm5(ind1)-arm5(ind1-1)-1);
            inantiwin = inantiwin + (arm3(ind1-1)-arm3(ind1)-1)*partonwin;
        else
            partonwin = (arm5(ind1)-winstart5)/(arm5(ind1)-1);
            inantiwin = inantiwin + (length(bulges)-arm3(ind1))*partonwin;
        end
    end
    if(bulges_win(end))
        partonwin = (win_end-arm5(ind2))/(arm5(ind2+1)-arm5(ind2)-1);
        inantiwin = inantiwin + (arm3(ind2)-arm3(ind2+1)-1)*partonwin;
    end
    sym_in_win = inwin-inantiwin;
    sym_out = bulged5-bulged3-sym_in_win;
else
    tt=find(arm3-winstart5 >= 0);
    ind1=tt(end); % index in arm3 of first base in win that is paired
    antiend = arm5(ind1);
    tt=find(arm3-win_end <= 0);
    ind2=tt(1); % index in arm3 of last base in win that is paired
    antistart = arm5(ind2);
    inantiwin = sum(bulges(antistart:antiend)); % without bulges at ends of anti
    if(bulges_win(1))
        partonwin = (arm3(ind1)-winstart5)/(arm3(ind1)-arm3(ind1+1)-1);
        inantiwin = inantiwin + (arm5(ind1+1)-arm5(ind1)-1)*partonwin;
    end
    if(bulges_win(end))
        if(ind2>1)
            partonwin = (win_end-arm3(ind2))/(arm3(ind2-1)-arm3(ind2)-1);
            inantiwin = inantiwin + (arm5(ind2)-arm5(ind2-1)-1)*partonwin;
        else
            partonwin = (win_end-arm3(ind2))/(length(bulges)-arm3(ind2));

```

```

    inantiwin = inantiwin + (arm5(ind2)-1)*partonwin;
end
end

sym_in_win = inwin-inantiwin;
sym_out = bulged3-bulged5-sym_in_win;
end
function seqs = transform_format(seqs,format);
%seqs = transform_format(seqs,format);
% format is either 'int' or 'nuc'
%if format not given, toggle format from int<-> nuc
% note that assume all seqs are in same format initially
if(nargin==1)
    if all(isletter(seqs{1}))
        format = 'int';
    else
        format = 'nuc';
    end
end
end

if(strcmp(format,'nuc'))
    for i = 1:length(seqs)
        seqs{i} = int2nuc(seqs{i});
    end
elseif(strcmp(format,'int'))
    for i = 1:length(seqs)
        seqs{i} = nuc2int(seqs{i});
    end
else
    error('transform_format: format (if given) must be int or nuc');
end
return

```

```

function visualize_dicer_structure(seqd, filename)
%visualize_dicer_structure(seqd, filename)
% show dicer on zuker structure
%seqd is in int
Mxplen = 250; % maximal length of palindrom
fid = fopen(filename,'r');
seq_no = 0;
seqs = cell(0);
while ~feof(fid)
    seq_no = seq_no + 1
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    [seq1, bulge1, endbulge1] = get_features(structure);
    seqs{seq_no} = seq1;

```

```

pos = findstr(seqd{seq_no}, seq1)
if ~isempty(pos)
    lend = length(seqd{seq_no});
    % search on structure for pos
    [id,jd] = dicer_on_structure(pos, lend, structure);
else
    id = [];
    jd = [];
end

plot_structure(structure,id,jd);
pause

end
return
function [id,jd] = dicer_on_structure(pos, lend, structure)
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
dicercount = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        if count >=pos & count < pos + lend
            dicercount = dicercount+1;
            id(dicercount) = fl(1);
            jd(dicercount) = col;
        end
    end
end
end
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        if count >=pos & count < pos + lend
            dicercount = dicercount+1;
            id(dicercount) = fl(1) + 2;
            jd(dicercount) = col;
        end
    end
end
end
return
function plot_structure(structure,id,jd);
yscale = 1.5;
clf

```

```

hold on
axis equal
[j,k] = find(isletter(structure));
max_col = max(k);
axis([ 0 max(75,max_col) 0 5*yscale]);
for x = 1:max_col
    for y = 1:4
        text(x,yscale*y,structure(5-y,x)); % so upper appears on top
    end
end
for k = 1:length(id);
    H = text(jd(k),yscale*(5-id(k)),structure(id(k),jd(k)));
    set(H,'color',[1 0 0]);
end
return
function [seq, bulge, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge(count) = (fl == bulge_row);
    end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge));
pos = length(bulge);
while bulge(pos) == 1
    endbulge(pos) = 1;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge(count) = (fl == bulge_row);
    end
end

```

```

        endbulge(count) = 0;
    end
end
return

function visualize_dicer_structure_gidi(seqd, filename)
%visualize_dicer_structure(seqd, filename)
% show dicer on zucker structure
if(~exist('filename'))
    filename = 'c:\rosetta\data_baseline_13_4\zucker_draw_h121.txt';
end
Mxplen = 250; % maximal length of palindrom
fid = fopen(filename,'r');
seq_no = 0;
seqs = cell(0);
while ~feof(fid)
    seq_no = seq_no + 1
    structure = char(4,250);
    for i = 1:4
        line = fgetl(fid);
        structure(i,1:length(line)) = line;
    end
    [seq1, bulge1, endbulge1] = get_features(structure);
    seqs{seq_no} = seq1;
    pos = findstr(seqd{seq_no}, nuc2int4(seq1));
    if ~isempty(pos)
        lend = length(seqd{seq_no});
        % search on structure for pos
        [id,jd] = dicer_on_structure(pos, lend, structure);
    else
        id = [];
        jd = [];
    end

    plot_structure(structure,id,jd);
    pause

end
return
function [id,jd] = dicer_on_structure(pos, lend, structure)
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
dicercount = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        if count >=pos & count < pos + lend

```



```

        dicercount = dicercount+1;
        id(dicercount) = fl(1);
        jd(dicercount) = col;
    end
end
end
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        if count >=pos & count < pos + lend
            dicercount = dicercount+1;
            id(dicercount) = fl(1) + 2;
            jd(dicercount) = col;
        end
    end
end
end
return
function plot_structure(structure,id,jd);
yscale = 1.5;
clf
hold on
axis equal
[j,k] = find(isletter(structure));
max_col = max(k);
axis([ 0 max(75,max_col) 0 5*yscale]);
for x = 1:max_col
    for y = 1:4
        text(x,yscale*y,structure(5-y,x)); % so upper appears on top
    end
end
end
for k = 1:length(id);
    H = text(jd(k),yscale*(5-id(k)),structure(id(k),jd(k)));
    set(H,'color',[1 0 0]);
end
return
function [seq, bulge, endbulge] = get_features(structure)
% get sequence as well as bulge structure
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if ~isempty(fl)

```

```

        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge(count) = (fl == bulge_row);
    end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge));
pos = length(bulge);
while bulge(pos) == 1
    endbulge(pos) = 1;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
lwhalf = structure(3:4,:);
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge(count) = (fl == bulge_row);
        endbulge(count) = 0;
    end
end
return

```

```

function model = build_model(seqs,bulges1,bulges2,endbulges,energy,homology,...
    edist_pos,edist_score,two_stage_pos,two_stage_score,model)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% letters
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
p_nuc_no_eb = pal_letter_freq_individual(seqs);
model.means_letter_freq_no_eb = mean(p_nuc_no_eb);
model.stds_letter_freq_no_eb = std(p_nuc_no_eb);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% energy
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
model.mean_energy = mean(energy);
model.std_energy = std(energy);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% bulge (no bulge no eb)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
p_bulge = bulge_distribution(bulges1, bulges2, endbulges);
model.mean_nobulge_no_eb= mean(p_bulge(:,3));
model.std_nobulge_no_eb = std(p_bulge(:,3));
function p = bulge_distribution(bulges1, bulges2, endbulges)
% p(i,1) - freq of bulge of type 1.
% p(i,2) - freq of bulge of type 2.
% p(i,3) - freq of no bulge (sum is 1).
% does not take into account the endbulge
if(~iscell(bulges1))
    tt{1} = bulges1;
    bulges1 = tt;
    clear tt;
    tt{1} = bulges2;
    bulges2 = tt;
    clear tt;

tt{1} = endbulges;
    endbulges = tt;
    clear tt;
end
Ns = 3; % 3 states: 1 (bulge1) 2 (bulge2) 3 (no bulge)
n = length(bulges1);
p = zeros(n,Ns);
for i = 1:n
    eff_len = length(bulges1{i}) - sum(endbulges{i}); % effective length
    p(i,1) = sum(bulges1{i})/eff_len;
    p(i,2) = sum(bulges2{i})/eff_len;
    p(i,3) = 1- p(i,1)- p(i,2);

```

```

end
function h = entropy(p,base)
% function h = entropy(p,base)
% function h = entropy(p)
% computes the entropy of the distribution p in base base
% if no base is given assumes base 2
h = sum(-1*xlog2x(p));
if(nargin==2)
    h = h/log2(base);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

function y = xlog2x(x)
l = 1:length(x);
l0 = find(x==0);
y(l0) = 0;
l1 = setdiff(l,l0);
y(l1) = x(l1).*log2(x(l1));

function score = get_palgrade(seqs,bulges1,bulges2,endbulges,energy,homology,...
    edist_pos,edist_score,two_stage_pos,two_stage_score,model)
if(~iscell(seqs))
    tt{1} = seqs;
    seqs = tt; clear tt;
    tt{1} = bulges1;
    bulges1 = tt; clear tt;
    tt{1} = bulges2;
    bulges2 = tt; clear tt;
    tt{1} = endbulges;
    endbulges = tt; clear tt;
end
if(model.filter_by_min_complexity)
    complexity = pal_complexities(seqs,model.complexity_window_size);
    for i = 1:length(seqs);
        this_c = complexity{i};
        if(min(this_c)<model.complexity_min_min_allowed)
            score(i) = 0;
        else
            score(i) = get_this_grade(seqs{i},bulges1{i},bulges2{i},endbulges{i},energy(i),...
                homology(i),edist_pos(i),edist_score(i),two_stage_pos(i),two_stage_score(i),model);
        end
    end
else
    for i = 1:length(seqs);
        score(i) = get_this_grade(seqs{i},bulges1{i},bulges2{i},endbulges{i},energy(i),...
            homology(i),edist_pos(i),edist_score(i),two_stage_pos(i),two_stage_score(i),model);
    end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function score = get_this_grade(seq,b1,b2,eb,energy,homology,e_pos,e_score,t_pos,t_score,model)

```

```

% normalize weights to sum of 1 :
sum_ws = model.w_freq_A + model.w_freq_C + model.w_freq_T + model.w_freq_G + ...
    model.w_energy + model.w_pal_length + model.w_nobulge + model.w_homology;
w_freq_A = model.w_freq_A/sum_ws;
w_freq_C = model.w_freq_C/sum_ws;
w_freq_T = model.w_freq_T/sum_ws;
w_freq_G = model.w_freq_G/sum_ws;
w_energy = model.w_energy/sum_ws;
w_pal_length = model.w_pal_length/sum_ws;
w_nobulge = model.w_nobulge/sum_ws;
w_homology = model.w_homology/sum_ws;
letter_scores = get_let_scores_exp(seq,eb,model);
nobulge_score = get_nobulge_score(b1,b2,eb,model);
energy_score = get_energy_score(energy,model);
pallen = length(seq);
score = w_freq_A * letter_scores(1) + w_freq_C * letter_scores(2) + ...
w_freq_T * letter_scores(3) + w_freq_G * letter_scores(4) + ...
w_energy * energy_score + ...
w_pal_length * (pallen>model.min_pal_length & pallen<model.max_pal_length) + ...
w_nobulge * nobulge_score + w_homology * exp(-(homology-1)^2/model.homology_exp_beta);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function score = min_max_score(min_v,max_v,dir_flag,value)
if(dir_flag == 1) % the higher the better
    score = (value - min_v)/(max_v - min_v);
elseif(dir_flag == -1) % the lower the better
    score = 1 - ((value - min_v)/(max_v - min_v));
else
    error('min_max_score: dir_flag must be 1 or -1. aborting');
end
if(score<0)
    score = 0;
    warning('min_max_score: encountered value outside range getting neg score. truncating score to 0');
end
if(score>1)
    score = 1;
    warning('min_max_score: encountered value outside range getting score higher than 1. truncating score to 1');
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function s = get_let_scores_exp(seq,eb,model)
tt = find(eb);
eb_begin = tt(1);
eb_end = tt(end);
index_range = [1:eb_begin-1, eb_end+1:length(seq)];
c = zeros(1,4);
for j = index_range
    c(seq(j)) = c(seq(j)) + 1;
end
f = c/sum(c); % frequencies of letters

```

```

alpha = model.letter_freq_exp_alpha;
means = model.means_letter_freq_no_eb;
stds = model.stds_letter_freq_no_eb;
s = exp(-(f-means).^2./(sqrt(2*pi)*(alpha*stds).^2));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function s = get_nobulge_score(b1,b2,eb,model);
eff_len = length(b1) - sum(eb); % effective length
t1 = sum(b1)/eff_len;
t2 = sum(b2)/eff_len;
f = 1- t1- t2;
alpha = model.letter_freq_exp_alpha;
m = model.mean_nobulge_no_eb;
st = model.std_nobulge_no_eb;
s = exp(-(f-m).^2./(sqrt(2*pi)*(alpha*st).^2));
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function s = get_energy_score(energy,model);
alpha = model.energy_exp_alpha;
m = model.mean_energy;
st = model.std_energy;
s = exp(-(energy-m).^2./(sqrt(2*pi)*(alpha*st).^2));
% homology = nan is considered 0 for histogram.
% also scores of edist and 2stage nan is taken as 0
paramfile = 'params5A';
set_name = 'hmdc440_sanger_09_09_03';
fid_k = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '.txt'],'r');
[seqs_k,anti_inds_k,bulges1_k,bulges2_k,endbulges_k,pal_id_k,energy_k,all_pal_ids_k] = ...
    read_structure_with_id_fid_ce(fid_k,1000);
fclose(fid_k);
if(length(pal_id_k)~=length(all_pal_ids_k))
    error('in animals data do not allow faulty seqs, take out of there');
end
% load the corresponding data cleaning the lines of faulty seqs. note that no edist and 2stage there
%data_k_tmp = load(['c:\rosetta\palgrade\pal_data\data_' set_name '.txt']);
%ids_tmp = data_k_tmp(:,1);
%if(length(ids_tmp)~=length(all_pal_ids_k) | any(ids_tmp(:)-all_pal_ids_k(:)))
%    error('ids in zucker file and data file must be identical and in the same order');
%end
%l = find(ismember(ids_tmp,pal_id_k));
%data_k = data_k_tmp(l,:);
%homology_k = data_k(:,7); % homology degree (nan means found no homology)
%nan_inds = find(isnan(homology_k));
%hom_inds_k = setdiff([1:length(homology_k)],nan_inds);
%homology_k(nan_inds) = 0;
% load the 2stage and edist pos and scores
%tt = load(['c:\rosetta\palgrade\pal_data\twostage_pos_score_' set_name '.txt']);
%two_stage_pos_k = tt(:,2);
%two_stage_score_k = tt(:,3);
%nan_inds = find(isnan(two_stage_score_k));

```

```

%two_stage_score_k(nan_inds) = 0;
%tt = load(['c:\rosetta\palgrade\pal_data\edist_pos_score_' set_name '.txt']);
%edist_pos_k = tt(:,2);
%edist_score_k = tt(:,3);
%nan_inds = find(isnan(edist_score_k));
%edist_score_k(nan_inds) = 0;
homology_k = zeros(1,length(pal_id_k));
two_stage_pos_k = zeros(1,length(pal_id_k));
two_stage_score_k = zeros(1,length(pal_id_k));
edist_pos_k = zeros(1,length(pal_id_k));
edist_score_k = zeros(1,length(pal_id_k));
fid_500 = fopen('c:\rosetta\palgrade\pal_data\resDrawing_d500.txt','r');
[seqs_500,anti_inds_500,bulges1_500,bulges2_500,endbulges_500,pal_id_500,energy_500,all_pal_ids_500] = ...
    OLDread_struct_ce(fid_500,1000);
fclose(fid_500);
% load the corresponding data cleaning the lines of faulty seqs
data_500_tmp = load('c:\rosetta\palgrade\pal_data\data_500.txt');
ids_tmp = data_500_tmp(:,1);
if(length(ids_tmp)~=length(all_pal_ids_500) | any(ids_tmp(:)-all_pal_ids_500(:)))
    error('ids in zucker file and data file must be identical and in the same order');
end
I = find(ismember(ids_tmp,pal_id_500));
data_500 = data_500_tmp(I,:);
two_stage_pos_500 = data_500(:,3);
two_stage_score_500 = data_500(:,4);
nan_inds = find(isnan(two_stage_score_500));
two_stage_score_500(nan_inds) = 0;
edist_pos_500 = data_500(:,5);
edist_score_500 = data_500(:,6);
nan_inds = find(isnan(edist_score_500));
edist_score_500(nan_inds) = 0;
homology_500 = data_500(:,7); % homology degree (nan means found no homology)
nan_inds = find(isnan(homology_500));
hom_inds_500 = setdiff([1:length(homology_500)],nan_inds);
homology_500(nan_inds) = 0;
load('c:\rosetta\palgrade\pal_data\chip_adil_len_above_60_saved_data.mat');
eval(paramfile);
model = model_params;
model = build_model(seqs_k,bulges1_k,bulges2_k,...
    endbulges_k,energy_k,homology_k,edist_pos_k,edist_score_k,two_stage_pos_k,...
    two_stage_score_k,model);
[score_500] = get_palgrade(seqs_500,bulges1_500,bulges2_500,...
    endbulges_500,energy_500,homology_500,edist_pos_500,edist_score_500,two_stage_pos_500,...
    two_stage_score_500,model);
[score_chip] = get_palgrade(seqs_chip,bulges1_chip,bulges2_chip,...
    endbulges_chip,energy_chip,homology_chip,edist_pos_chip,edist_score_chip,two_stage_pos_chip,...
    two_stage_score_chip,model);
mfold = 3;
group_size = round(length(homology_k)/mfold);
perm_vec = randperm(length(homology_k));

```

```

clear score_known;
for i=1:mfold
    test_inds = perm_vec((i-1)*group_size + 1 : min(length(perm_vec),i*group_size));
    train_inds = setdiff(perm_vec,test_inds);

    clear model;
    eval(paramfile);
    model = model_params;

    model = build_model(seqs_k(train_inds),bulges1_k(train_inds),bulges2_k(train_inds),...
        endbulges_k(train_inds),energy_k(train_inds),homology_k(train_inds),edist_pos_k(train_inds),...
        edist_score_k(train_inds),two_stage_pos_k(train_inds),...
        two_stage_score_k(train_inds),model);

    [score_known(test_inds)] = get_palgrade(seqs_k(test_inds),bulges1_k(test_inds),...
        bulges2_k(test_inds),endbulges_k(test_inds),energy_k(test_inds),homology_k(test_inds),...
        edist_pos_k(test_inds),edist_score_k(test_inds),two_stage_pos_k(test_inds),...
        two_stage_score_k(test_inds),model);
end

hist_vec = [0:0.05:1];
cos1 = 0.75;
cos2 = 0.8;
[n_known,x] = hist(score_known,hist_vec);
n_known_norm = n_known/sum(n_known);
[n_500,x] = hist(score_500,hist_vec);
n_500_norm = n_500/sum(n_500);
[n_chip,x] = hist(score_chip,hist_vec);
n_chip_norm = n_chip/sum(n_chip);
figure;
plot(x,n_known_norm,'b-o',x,n_500_norm,'r-*',x,n_chip_norm,'k-*','linewidth',2);
axis_vec = [min(hist_vec), max(hist_vec), 0 ,0.2];
axis(axis_vec);
legend('known','500','chip');
tt = axis_vec(end);
j = tt/15;
text(0.1,tt-j,['mean known: ' num2str(mean(score_known))]);
text(0.1,tt-2*j,['mean 500: ' num2str(mean(score_500))]);
text(0.1,tt-3*j,['mean chip: ' num2str(mean(score_chip))]);
text(0.1,tt-5*j,['num >= ' num2str(cos1) ' known: ' num2str(sum(score_known>=cos1))]);
text(0.1,tt-6*j,['num >= ' num2str(cos1) ' 500: ' num2str(sum(score_500>=cos1))]);
text(0.1,tt-7*j,['num >= ' num2str(cos1) ' chip: ' num2str(sum(score_chip>=cos1))]);
text(0.1,tt-9*j,['num >= ' num2str(cos2) ' known: ' num2str(sum(score_known>=cos2))]);
text(0.1,tt-10*j,['num >= ' num2str(cos2) ' 500: ' num2str(sum(score_500>=cos2))]);
text(0.1,tt-11*j,['num >= ' num2str(cos2) ' chip: ' num2str(sum(score_chip>=cos2))]);
fid = fopen('info_and_criteria.txt','w');
fprintf(fid,'%sthresh,num knowns passing it,in perc,num of 500 passing it,in perc,\n\n');
fprintf(fid,'%snum of chip passing it\n\n');
thresh_vec=[0:0.01:1];
n_known = length(score_known);
n_500 = length(score_500);

```



```

n_chip = length(score_chip);
for i=1:length(thresh_vec)
    thresh = thresh_vec(i);
    c_known = sum(score_known>=thresh);
    r_known = c_known/n_known;
    c_500 = sum(score_500>=thresh);
    r_500 = c_500/n_500;
    c_chip = sum(score_chip>=thresh);
    r_chip = c_chip/n_chip;
    fprintf(fid,'%g\t%g\t%g\t%g\t%g\t%g\t%g\n',thresh,c_known,r_known,c_500,r_500,c_chip,r_chip);
end
fclose(fid);
save measure_perf_rundata.mat
% homology = nan is considered 0 for histogram.
% also scores of edist and 2stage nan is taken as 0
if(~exist('mfold'));
    mfold = 3;
end
paramfile = 'params_tests';
load_data = 0;
if(load_data)
    % load human knowns data
    set_name = 'h152';
    fid_k = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '.txt'],'r');
    [seqs_k,anti_inds_k,bulges1_k,bulges2_k,endbulges_k,pal_id_k,energy_k,all_pal_ids_k] = ...
        read_structure_with_id_fid(fid_k,1000);
    fclose(fid_k);
    if(length(pal_id_k)~=length(all_pal_ids_k))
        error('in human data do not allow faulty seqs, take out of there');
    end
    % load the corresponding data cleaning the lines of faulty seqs. note that no edist and 2stage there
    data_k_tmp = load(['c:\rosetta\palgrade\pal_data\data_' set_name '_blat.txt']);
    ids_tmp = data_k_tmp(:,1);
    if(length(ids_tmp)~=length(all_pal_ids_k) | any(ids_tmp(:)-all_pal_ids_k(:)))
        error('ids in zucker file and data file must be identical and in the same order');
    end
    I = find(ismember(ids_tmp,pal_id_k));
    data_k = data_k_tmp(I,:);
    homology_k = data_k(:,7); % homology degree (nan means found no homology)
    nan_inds = find(isnan(homology_k));
    hom_inds_k = setdiff([1:length(homology_k)],nan_inds);
    homology_k(nan_inds) = 0;
    % load the 2stage and edist pos and scores
    %tt = load(['c:\rosetta\palgrade\pal_data\twostage_pos_score_' set_name '.txt']);
    %two_stage_pos_k = tt(:,2);
    %two_stage_score_k = tt(:,3);
    %nan_inds = find(isnan(two_stage_score_k));
    %two_stage_score_k(nan_inds) = 0;
    %tt = load(['c:\rosetta\palgrade\pal_data\edist_pos_score_' set_name '.txt']);
    %edist_pos_k = tt(:,2);

```

```

%edist_score_k = tt(:,3);
%nan_inds = find(isnan(edist_score_k));
%edist_score_k(nan_inds) = 0;
two_stage_pos_k = zeros(1,length(pal_id_k));
two_stage_score_k = zeros(1,length(pal_id_k));
edist_pos_k = zeros(1,length(pal_id_k));
edist_score_k = zeros(1,length(pal_id_k));
% load a smaple of 500 pals
fid_500 = fopen('c:\rosetta\palgrade\pal_data\resDrawing_d500.txt','r');
[seqs_500,anti_inds_500,bulges1_500,bulges2_500,endbulges_500,pal_id_500,energy_500,all_pal_ids_500] = ...
    read_structure_with_id_fid(fid_500,1000);
fclose(fid_500);
% load the corresponding data cleaning the lines of faulty seqs
data_500_tmp = load('c:\rosetta\palgrade\pal_data\data_500.txt');
ids_tmp = data_500_tmp(:,1);
if(length(ids_tmp)~=length(all_pal_ids_500) | any(ids_tmp(:)-all_pal_ids_500(:)))
    error('ids in zuker file and data file must be identical and in the same order');
end
I = find(ismember(ids_tmp,pal_id_500));
data_500 = data_500_tmp(I,:);
two_stage_pos_500 = data_500(:,3);
two_stage_score_500 = data_500(:,4);
nan_inds = find(isnan(two_stage_score_500));
two_stage_score_500(nan_inds) = 0;
edist_pos_500 = data_500(:,5);
edist_score_500 = data_500(:,6);
nan_inds = find(isnan(edist_score_500));
edist_score_500(nan_inds) = 0;
homology_500 = data_500(:,7); % homology degree (nan means found no homology)
nan_inds = find(isnan(homology_500));
hom_inds_500 = setdiff([1:length(homology_500)],nan_inds);
homology_500(nan_inds) = 0;

% load a smaple of 500 pals under 8 in old palgrade
fid_500_Under8 = fopen('c:\rosetta\palgrade\pal_data\resDrawing_d500_Under8.txt','r');
[seqs_500_Under8,anti_inds_500_Under8,bulges1_500_Under8,bulges2_500_Under8,...
    endbulges_500_Under8,pal_id_500_Under8,energy_500_Under8,all_pal_ids_500_Under8] = ...
    read_structure_with_id_fid(fid_500_Under8,1000);
fclose(fid_500_Under8);
% load the corresponding data cleaning the lines of faulty seqs
data_500_Under8_tmp = load('c:\rosetta\palgrade\pal_data\data_500_Under8.txt');
ids_tmp = data_500_Under8_tmp(:,1);
if(length(ids_tmp)~=length(all_pal_ids_500_Under8) | any(ids_tmp(:)-all_pal_ids_500_Under8(:)))
    error('ids in zuker file and data file must be identical and in the same order');
end
I = find(ismember(ids_tmp,pal_id_500_Under8));
data_500_Under8 = data_500_Under8_tmp(I,:);
two_stage_pos_500_Under8 = data_500_Under8(:,3);
two_stage_score_500_Under8 = data_500_Under8(:,4);
nan_inds = find(isnan(two_stage_score_500_Under8));

```

```

two_stage_score_500_under8(nan_inds) = 0;
edist_pos_500_Under8 = data_500_Under8(:,5);
edist_score_500_Under8 = data_500_Under8(:,6);
nan_inds = find(isnan(edist_score_500_Under8));
edist_score_500_under8(nan_inds) = 0;
homology_500_Under8 = data_500_Under8(:,7); % homology degree (nan means found no homology)
nan_inds = find(isnan(homology_500_Under8));
hom_inds_500_Under8 = setdiff([1:length(homology_500_Under8)],nan_inds);
homology_500_Under8(nan_inds) = 0;

load('c:\rosetta\palgrade\pal_data\chip_adi_len_above_60_saved_data.mat');
end
%for known do mfold
%group_size = round(length(pal_id_k)/mfold);
%perm_vec = randperm(length(pal_id_k));
group_size = round(length(homology_k)/mfold);
perm_vec = randperm(length(homology_k));
clear score_known;
for i=1:mfold
    test_inds = perm_vec((i-1)*group_size + 1 : min(length(perm_vec),i*group_size));
    train_inds = setdiff(perm_vec,test_inds);

    clear model;
    eval(paramfile);
    model = model_params;

    model = build_model(seqs_k(train_inds),bulges1_k(train_inds),bulges2_k(train_inds),...
        endbulges_k(train_inds),energy_k(train_inds),homology_k(train_inds),edist_pos_k(train_inds),...
        edist_score_k(train_inds),two_stage_pos_k(train_inds),...
        two_stage_score_k(train_inds),model);

    [score_known(test_inds)] = get_palgrade(seqs_k(test_inds),bulges1_k(test_inds),...
        bulges2_k(test_inds),endbulges_k(test_inds),energy_k(test_inds),homology_k(test_inds),...
        edist_pos_k(test_inds),edist_score_k(test_inds),two_stage_pos_k(test_inds),...
        two_stage_score_k(test_inds),model);
end
% for unknowns use all knowns to predict
clear model;
eval(paramfile);
model = model_params;
model = build_model(seqs_k,bulges1_k,bulges2_k,...
    endbulges_k,energy_k,homology_k,edist_pos_k,edist_score_k,two_stage_pos_k,...
    two_stage_score_k,model);
[score_500] = get_palgrade(seqs_500,bulges1_500,bulges2_500,...
    endbulges_500,energy_500,homology_500,edist_pos_500,edist_score_500,two_stage_pos_500,...
    two_stage_score_500,model);
[score_500_Under8] = get_palgrade(seqs_500_Under8,bulges1_500_Under8,bulges2_500_Under8,...
    endbulges_500_Under8,energy_500_Under8,homology_500_Under8,edist_pos_500_Under8,...
    edist_score_500_Under8,two_stage_pos_500_Under8,two_stage_score_500_Under8,model);
[score_chip] = get_palgrade(seqs_chip,bulges1_chip,bulges2_chip,...

```

```

endbulges_chip,energy_chip,homology_chip,edist_pos_chip,edist_score_chip,two_stage_pos_chip,...
two_stage_score_chip,model);
hist_vec = [0:0.05:1];
cos1 = 0.75;
cos2 = 0.8;
[n_known,x] = hist(score_known,hist_vec);
n_known_norm = n_known/sum(n_known);
[n_500,x] = hist(score_500,hist_vec);
n_500_norm = n_500/sum(n_500);
[n_chip,x] = hist(score_chip,hist_vec);
n_chip_norm = n_chip/sum(n_chip);
figure;
plot(x,n_known_norm,'b-o',x,n_500_norm,'r-*',x,n_chip_norm,'k-*','linewidth',2);
axis_vec = [min(hist_vec), max(hist_vec), 0 ,0.2];
axis(axis_vec);
legend('known human','500','chip');
tt = axis_vec(end);
j = tt/15;
text(0.1,tt-j,['mean known: ' num2str(mean(score_known))]);
text(0.1,tt-2*j,['mean 500: ' num2str(mean(score_500))]);
text(0.1,tt-3*j,['mean chip: ' num2str(mean(score_chip))]);
text(0.1,tt-5*j,['num >= ' num2str(cos1) ' known: ' num2str(sum(score_known>=cos1))]);
text(0.1,tt-6*j,['num >= ' num2str(cos1) ' 500: ' num2str(sum(score_500>=cos1))]);
text(0.1,tt-7*j,['num >= ' num2str(cos1) ' chip: ' num2str(sum(score_chip>=cos1))]);
text(0.1,tt-9*j,['num >= ' num2str(cos2) ' known: ' num2str(sum(score_known>=cos2))]);
text(0.1,tt-10*j,['num >= ' num2str(cos2) ' 500: ' num2str(sum(score_500>=cos2))]);
text(0.1,tt-11*j,['num >= ' num2str(cos2) ' chip: ' num2str(sum(score_chip>=cos2))]);
function [intseq, fault_seq] = nuc2int4_new(strseq);
%[intseq, fault_seq] = nuc2int4_new(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
intseq = zeros(size(strseq));
fault_seq = 0;
for i = 1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i) = 1;
        case 'C' , intseq(i) = 2;
        case 'T' , intseq(i) = 3;
        case 'G' , intseq(i) = 4;
        otherwise , intseq = []; fault_seq = 1; break;
    end
end
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
% in this check_e version returns faulty seq also when no energy found

```

```

Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
next_pal_id = str2double(fgetl(fid));
while ~feof(fid) & seq_no < seqtot
    this_pal_id = next_pal_id;
    this_energy = str2double(fgetl(fid));
    if(isnan(this_energy))
        fault_seq_energy = 1;
    else
        fault_seq_energy = 0;
    end
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    fault_seq_emptyline = 0;
    while((line~-1 & isnan(str2double(line))) | isempty(line))
        if(isempty(line))
            fault_seq_emptyline = 1;
        end
        i = i+1;
        structure(i,1:length(line)) = line;
        line = fgetl(fid);
    end
    if(~feof(fid))
        next_pal_id = str2double(line);
    end
    if(i~=4)
        fault_seq_numlines = 1;
    else
        fault_seq_numlines = 0;
    end

    fault_seq_struct = 1; % guilty until proven innocent
    fault_seq_nuc = 1;
    if(fault_seq_numlines == 0 & fault_seq_emptyline==0 & fault_seq_energy==0)
        [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
        if(fault_seq_struct==0)
            % this is the old bulge1 and bulge2, now need to correct that
            bulge_nonsymi=bulge1i;
            bulge_symi=bulge2i;
            for j = 1:length(seqi)
                if(bulge_nonsymi(j))
                    if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on

```

```

        bulge_symi(j) = 1;
        bulge_nonsymi(j) = 0;
    end
end
end
for j = length(seqi):-1:1
    if(bulge_nonsymi(j))
        if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
            bulge_symi(j) = 1;
            bulge_nonsymi(j) = 0;
        end
    end
end
end
[intseq, fault_seq_nuc] = nuc2int4_new(seqi);
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0 &
fault_seq_energy==0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    if(fault_seq_energy)
        disp(['reason is that there was no energy']);
    elseif(fault_seq_emptyline)
        disp(['reason is that there was an empty line in zucker']);
    elseif(fault_seq_numlines)
        disp(['reason is that there were not 4 lines in the draw']);
    elseif(fault_seq_struct)
        disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
    elseif(fault_seq_nuc)
        disp(['reason is that there was an illegal letter in the seq']);
    end
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)

```

```

% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col = 1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1);
        fault_seq = 1;
        seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
        return;
    end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);

```

```

for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function c = pal_complexities(seqs,winsize,endbulges)
%c = pal_complexities(seqs,winsize,endbulges)
%c = pal_complexities(seqs,winsize)
%second version looks also at endbulge, first ignores the letters there
%c is a cell array where c{i} is a vector holding the complexity measures of
% all windows fitting in the seq of the ith pal
Ns = 4; %number of states
if nargin == 3
    omit_endbulge = 1;
else
    omit_endbulge = 0;
end
%test if single sequence
if ~iscell(seqs)
    t = cell(1);
    t{1} = seqs;
    seqs = t;
    if omit_endbulge == 1
        t = cell(1);
        t{1} = endbulges;
        endbulges = t;
    end
end

```



```

end
clear t
end
c = cell(0);
for i = 1:length(seqs)
    this_c = [];
    seqsi = seqs{i};
    if omit_endbulge
        eb = find(endbulges{i});
        eb_begin = eb(1);
        eb_end = eb(end);
        for j=1:eb_begin-1-(winsize-1)
            this_winseq = seqsi(j:j+winsize-1);
            this_c = [this_c,get_seq_complexity(this_winseq)];
        end
        for j=eb_end+1:length(seqsi)-(winsize-1)
            this_winseq = seqsi(j:j+winsize-1);
            this_c = [this_c,get_seq_complexity(this_winseq)];
        end
    else
        for j=1:length(seqsi)-(winsize-1)
            this_winseq = seqsi(j:j+winsize-1);
            this_c = [this_c,get_seq_complexity(this_winseq)];
        end
    end
    c{i} = this_c;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function c = get_seq_complexity(seq)
p = zeros(1,4);
for j=1:length(seq)
    p(seq(j)) = p(seq(j)) + 1;
end
p = p/sum(p); % letter freq in this seq
c = entropy(p); % complexity is simply the entropy of the seq in the window

function p = pal_letter_freq_individual(seqs,endbulges)
%p = pal_letter_freq_individual(seqs,endbulges)
%p = pal_letter_freq_individual(seqs)
%second version looks also at endbulge, first ignores the letters there
%p is a matrix of size numseqs by 4. p(i,:) is the frequencies of the 4 letters
%in the ith palindrom
Ns = 4; %number of states
if nargin == 2
    omit_endbulge = 1;
else
    omit_endbulge = 0;
end
%test if single sequence

```

```

if ~iscell(seqs)
    t = cell(1);
    t{1} = seqs;
    seqs = t;
    if omit_endbulge == 1
        t = cell(1);
        t{1} = endbulges;
        endbulges = t;
    end
    clear t
end
p = zeros(length(seqs),Ns);
for i = 1:length(seqs)
    seqsi = seqs{i};
    if omit_endbulge
        eb = find(endbulges{i});
        eb_begin = min(eb);
        eb_end = max(eb);
        index_range = [1:eb_begin-1 eb_end+1:length(seqsi)];
    else
        index_range = [1:length(seqsi)];
    end
    %1 gram
    c1i = zeros(1,Ns);
    for j = index_range
        c1i(seqsi(j)) = c1i(seqsi(j)) + 1;
    end
    p(i,:) = c1i/sum(c1i);
end

% general
model_params.data_used_for_known_pals = 'animals 441 from sanger 09 September 2003';
% below the weights of each feature in the total score. The score of
% a palindrom is the sum of each of the individual scores times its
% weight. system normalizes the sum of these to 1 (so here take care only of ratios)
model_params.w_freq_A = 0.25;
model_params.w_freq_C = 0.25;
model_params.w_freq_T = 0.25;
model_params.w_freq_G = 0.5;
model_params.w_energy = 1;
model_params.w_pal_length = 0.75;
model_params.w_nobulge = 0.25;
model_params.w_homology = 0;
% letter freq stuff. uses freq of nucs not in endbulge. order is A,C,T,G.
% uses exp such that the score at the mean is 1.  $\exp((f-m)^2/(\text{sqrt}(2\pi)*(\alpha*s)^2))$ 
% m is the mean and s the std of the knowns.
model_params.letter_freq_exp_alpha = 0.7;
% complexity stuff. if filter_by_min_complexity=1 filters by complexity.
% runs on windows of size complexity_window_size and computes the
% entropy in that window. Then looks for each pal at the minimal entropy

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% in all of its windows. If that is less than complexity_min_min_allowed
% gives a score of 0 to that pal. else goes on as usual.
model_params.filter_by_min_complexity = 1;
model_params.complexity_window_size = 10;
model_params.complexity_min_min_allowed = 0.7;
% energy stuff. score is a exp as for letter freq.
model_params.energy_exp_alpha = 0.7;
% pal length stuff. score is 1 inside win and 0 outside.
model_params.min_pal_length = 70;
model_params.max_pal_length = 115;
% bulge stuff. uses ratio of no bulges (like ratio of paired)
% doesnt take into account the endbulge
% uses  $\exp((f-m)^2/(\text{sqrt}(2\pi)*(\alpha*s)^2))$ 
% m is the mean and s the std of the knowns.
model_params.nobulge_exp_alpha = 0.7;
% homology stuff
% uses  $\exp(-(h-1).^2/\beta)$ ;
model_params.homology_exp_beta = 0.02;
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid_ce(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
% in this check_e version returns faulty seq also when no energy found
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
while ~feof(fid) & seq_no < seqtot
    this_pal_id = str2double(fgetl(fid));
    this_energy = str2double(fgetl(fid));
    if(isnan(this_energy))
        fault_seq_energy = 1;
    else
        fault_seq_energy = 0;
    end
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    if isempty(line)
        line = 'emptyline';
        fault_seq_emptyline = 1;
    end
end

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else
    fault_seq_emptyline = 0;
end
while(line(1)~='|') % if emptyline this is always true so will go into loop
    i = i+1;
    structure(i,1:length(line)) = line;
    line = fgetl(fid);
    if isempty(line)
        line = 'emptyline';
        fault_seq_emptyline = 1;
    end
end
if(i~=4)
    fault_seq_numlines = 1;
else
    fault_seq_numlines = 0;
end

fault_seq_struct = 1; % guilty until proven innocent
fault_seq_nuc = 1;
if(fault_seq_numlines == 0 & fault_seq_emptyline==0 & fault_seq_energy==0)
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
    if(fault_seq_struct==0)
        % this is the old bulge1 and bulge2, now need to correct that
        bulge_nonsymi=bulge1i;
        bulge_symi=bulge2i;
        for j = 1:length(seqi)
            if(bulge_nonsymi(j))
                if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        for j = length(seqi):-1:1
            if(bulge_nonsymi(j))
                if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        [intseq, fault_seq_nuc] = nuc2int4_new(seqi);
    end
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0 &
fault_seq_energy==0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
end

```

```

anti_inds{seq_no} = anti_indi;
bulges_nonsym{seq_no} = bulge_nonsymi;
bulges_sym{seq_no} = bulge_symi;
endbulges{seq_no} = endbulgei;
pal_id(seq_no) = this_pal_id;
energy(seq_no) = this_energy;
counter = counter + 1;
all_pal_ids(counter) = this_pal_id;
else
disp(['faulty seq on pal id ' num2str(this_pal_id)])
if(fault_seq_energy)
disp(['reason is that there was no energy']);
elseif(fault_seq_emptyline)
disp(['reason is that there was an empty line in zucker']);
elseif(fault_seq_numlines)
disp(['reason is that there were not 4 lines in the draw']);
elseif(fault_seq_struct)
disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
elseif(fault_seq_nuc)
disp(['reason is that there was an illegal letter in the seq']);
end
counter = counter + 1;
all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col = 1: max_col
fl = find(isletter(uphalf(:,col))));
if (length(fl)>1);
fault_seq = 1;
seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
return;
end;
if ~isempty(fl)
count = count + 1;
seq(count) = uphalf(fl,col);
bulge = (fl == bulge_row);

```

```

    if(bulge)
        tmpmat(1,col) = 0;
    else
        tmpmat(1,col) = count;
    end
    bulge1(count) = 0;
    bulge2(count) = 0;
    if bulge & isletter(structure(bulge_row_opposite,col))
        bulge2(count) = 1;
    elseif bulge & ~isletter(structure(bulge_row_opposite,col))
        bulge1(count) = 1;
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));
lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col =max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
end
end

```

```

anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function run_palgrade()
zucker_filename = 'XXX';
data_filename = 'XXX';
output_filename = 'XXX';
load model_palgrade5A_a441;
fidin = fopen(zucker_filename,'r');
fidout = fopen(output_filename,'w');
fidindata = fopen(data_filename,'r');
seqstot = 1000; %number of sequences to classify each loop
while ~feof(fidin)
    disp('reading structure...');

    [seqs,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
        read_structure_with_id_fid_ce(fidin,seqstot);
    % load the corresponding data cleaning the lines of faulty seqs
    clear data_tmp;
    for i=1:length(all_pal_ids)
        data_tmp(i,:) = str2num(fgetl(fidindata));
    end
    ids_tmp = data_tmp(:,1);
    if(length(ids_tmp)~=length(all_pal_ids) | any(ids_tmp(:)-all_pal_ids(:)))
        error('ids in zucker file and data file must be identical and in the same order');
    end
    I = find(ismember(ids_tmp,pal_id));
    data = data_tmp(I,:);
    two_stage_pos = data(:,3);
    two_stage_score = data(:,4);
    nan_inds = find(isnan(two_stage_score));
    two_stage_score(nan_inds) = 0;
    edist_pos = data(:,5);
    edist_score = data(:,6);
    nan_inds = find(isnan(edist_score));
    edist_score(nan_inds) = 0;
    homology = data(:,7); % homology degree (nan means found no homology)
    nan_inds = find(isnan(homology));
    hom_inds = setdiff([1:length(homology)],nan_inds);
    homology(nan_inds) = 0;

    score = get_palgrade(seqs,bulges1,bulges2,endbulges,energy,homology,...
        edist_pos,edist_score,two_stage_pos,two_stage_score,model);

    for i = 1:length(score)

```

```

        fprintf(fidout,'%d\t%g\t',pal_id(i),score(i));
    end
end
fclose(fidin);
fclose(fidindata);
fclose(fidout)
function run_palgrade_for_tests(zuker_filename,data_filename,output_filename)
load model_palgrade5A_a441;
fidin = fopen(zuker_filename,'r');
fidout = fopen(output_filename,'w');
fidindata = fopen(data_filename,'r');
seqstot = 1000; %number of sequences to classify each loop
while ~feof(fidin)
    disp('reading structure...');
    [seqs,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
        read_structure_with_id_fid_ce(fidin,seqstot);
    % load the corresponding data cleaning the lines of faulty seqs
    clear data_tmp;
    for i=1:length(all_pal_ids)
        data_tmp(i,:) = str2num(fgetl(fidindata));
    end
    ids_tmp = data_tmp(:,1);
    if(length(ids_tmp)~=length(all_pal_ids) | any(ids_tmp(:)-all_pal_ids(:)))
        error('ids in zuker file and data file must be identical and in the same order');
    end
    I = find(ismember(ids_tmp,pal_id));
    data = data_tmp(I,:);
    two_stage_pos = data(:,3);
    two_stage_score = data(:,4);
    nan_inds = find(isnan(two_stage_score));
    two_stage_score(nan_inds) = 0;
    edist_pos = data(:,5);
    edist_score = data(:,6);
    nan_inds = find(isnan(edist_score));
    edist_score(nan_inds) = 0;
    homology = data(:,7); % homology degree (nan means found no homology)
    nan_inds = find(isnan(homology));
    hom_inds = setdiff([1:length(homology)],nan_inds);
    homology(nan_inds) = 0;

    score = get_palgrade(seqs,bulges1,bulges2,endbulges,energy,homology,...
        edist_pos,edist_score,two_stage_pos,two_stage_score,model);

    for i = 1:length(score)
        fprintf(fidout,'%d\t%g\t',pal_id(i),score(i));
    end
end
fclose(fidin);
fclose(fidindata);
fclose(fidout)

```



```

% homology = nan is considered 0 for histogram.
% also scores of edist and 2stage nan is taken as 0
paramfile = 'params5A';
set_name = 'a441_sanger_09_09_03';
fid_k = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '.txt'],'r');
[seqs_k,anti_inds_k,bulges1_k,bulges2_k,endbulges_k,pal_id_k,energy_k,all_pal_ids_k] = ...
    read_structure_with_id_fid_ce(fid_k,1000);
fclose(fid_k);
if(length(pal_id_k)~=length(all_pal_ids_k))
    error('in animals data do not allow faulty seqs, take out of there');
end
% load the corresponding data cleaning the lines of faulty seqs. note that no edist and 2stage there
data_k_tmp = load(['c:\rosetta\palgrade\pal_data\data_' set_name '.txt']);
ids_tmp = data_k_tmp(:,1);
if(length(ids_tmp)~=length(all_pal_ids_k) | any(ids_tmp(:)-all_pal_ids_k(:)))
    error('ids in zucker file and data file must be identical and in the same order');
end
I = find(ismember(ids_tmp,pal_id_k));
data_k = data_k_tmp(I,:);
homology_k = data_k(:,7); % homology degree (nan means found no homology)
nan_inds = find(isnan(homology_k));
hom_inds_k = setdiff([1:length(homology_k)],nan_inds);
homology_k(nan_inds) = 0;
% load the 2stage and edist pos and scores
%tt = load(['c:\rosetta\palgrade\pal_data\twostage_pos_score_' set_name '.txt']);
%two_stage_pos_k = tt(:,2);
%two_stage_score_k = tt(:,3);
%nan_inds = find(isnan(two_stage_score_k));
%two_stage_score_k(nan_inds) = 0;
%tt = load(['c:\rosetta\palgrade\pal_data\edist_pos_score_' set_name '.txt']);
%edist_pos_k = tt(:,2);
%edist_score_k = tt(:,3);
%nan_inds = find(isnan(edist_score_k));
%edist_score_k(nan_inds) = 0;
two_stage_pos_k = zeros(1,length(pal_id_k));
two_stage_score_k = zeros(1,length(pal_id_k));
edist_pos_k = zeros(1,length(pal_id_k));
edist_score_k = zeros(1,length(pal_id_k));
fid_500 = fopen('c:\rosetta\palgrade\pal_data\resDrawing_d500.txt','r');
[seqs_500,anti_inds_500,bulges1_500,bulges2_500,endbulges_500,pal_id_500,energy_500,all_pal_ids_500] = ...
    OLDread_struct_ce(fid_500,1000);
fclose(fid_500);
% load the corresponding data cleaning the lines of faulty seqs
data_500_tmp = load('c:\rosetta\palgrade\pal_data\data_500.txt');
ids_tmp = data_500_tmp(:,1);
if(length(ids_tmp)~=length(all_pal_ids_500) | any(ids_tmp(:)-all_pal_ids_500(:)))
    error('ids in zucker file and data file must be identical and in the same order');
end
I = find(ismember(ids_tmp,pal_id_500));
data_500 = data_500_tmp(I,:);

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```

two_stage_pos_500 = data_500(:,3);
two_stage_score_500 = data_500(:,4);
nan_inds = find(isnan(two_stage_score_500));
two_stage_score_500(nan_inds) = 0;
edist_pos_500 = data_500(:,5);
edist_score_500 = data_500(:,6);
nan_inds = find(isnan(edist_score_500));
edist_score_500(nan_inds) = 0;
homology_500 = data_500(:,7); % homology degree (nan means found no homology)
nan_inds = find(isnan(homology_500));
hom_inds_500 = setdiff([1:length(homology_500)],nan_inds);
homology_500(nan_inds) = 0;
load('c:\rosetta\palgrade\pal_data\chip_adi_len_above_60_saved_data.mat');
eval(paramfile);
model = model_params;
model = build_model(seqs_k,bulges1_k,bulges2_k,...
    endbulges_k,energy_k,homology_k,edist_pos_k,edist_score_k,two_stage_pos_k,...
    two_stage_score_k,model);
save model_palgrade5A_a441 model
[score_500] = get_palgrade(seqs_500,bulges1_500,bulges2_500,...
    endbulges_500,energy_500,homology_500,edist_pos_500,edist_score_500,two_stage_pos_500,...
    two_stage_score_500,model);
[score_chip] = get_palgrade(seqs_chip,bulges1_chip,bulges2_chip,...
    endbulges_chip,energy_chip,homology_chip,edist_pos_chip,edist_score_chip,two_stage_pos_chip,...
    two_stage_score_chip,model);
mfold = 3;
group_size = round(length(homology_k)/mfold);
perm_vec = randperm(length(homology_k));
clear score_known;
for i=1:mfold
    test_inds = perm_vec((i-1)*group_size + 1 : min(length(perm_vec),i*group_size));
    train_inds = setdiff(perm_vec,test_inds);

    clear model;
    eval(paramfile);
    model = model_params;

    model = build_model(seqs_k(train_inds),bulges1_k(train_inds),bulges2_k(train_inds),...
        endbulges_k(train_inds),energy_k(train_inds),homology_k(train_inds),edist_pos_k(train_inds),...
        edist_score_k(train_inds),two_stage_pos_k(train_inds),...
        two_stage_score_k(train_inds),model);

    [score_known(test_inds)] = get_palgrade(seqs_k(test_inds),bulges1_k(test_inds),...
        bulges2_k(test_inds),endbulges_k(test_inds),energy_k(test_inds),homology_k(test_inds),...
        edist_pos_k(test_inds),edist_score_k(test_inds),two_stage_pos_k(test_inds),...
        two_stage_score_k(test_inds),model);
end
hist_vec = [0:0.05:1];
cos1 = 0.75;
cos2 = 0.8;

```

```

[n_known,x] = hist(score_known,hist_vec);
n_known_norm = n_known/sum(n_known);
[n_500,x] = hist(score_500,hist_vec);
n_500_norm = n_500/sum(n_500);
[n_chip,x] = hist(score_chip,hist_vec);
n_chip_norm = n_chip/sum(n_chip);
figure;
plot(x,n_known_norm,'b-o',x,n_500_norm,'r-*',x,n_chip_norm,'k-*','linewidth',2);
axis_vec = [min(hist_vec), max(hist_vec), 0 ,0.2];
axis(axis_vec);
legend('known','500','chip');
tt = axis_vec(end);
j = tt/15;
text(0.1,tt-j,['mean known: ' num2str(mean(score_known))]);
text(0.1,tt-2*j,['mean 500: ' num2str(mean(score_500))]);
text(0.1,tt-3*j,['mean chip: ' num2str(mean(score_chip))]);
text(0.1,tt-5*j,['num >= ' num2str(cos1) ' known: ' num2str(sum(score_known>=cos1))]);
text(0.1,tt-6*j,['num >= ' num2str(cos1) ' 500: ' num2str(sum(score_500>=cos1))]);
text(0.1,tt-7*j,['num >= ' num2str(cos1) ' chip: ' num2str(sum(score_chip>=cos1))]);
text(0.1,tt-9*j,['num >= ' num2str(cos2) ' known: ' num2str(sum(score_known>=cos2))]);
text(0.1,tt-10*j,['num >= ' num2str(cos2) ' 500: ' num2str(sum(score_500>=cos2))]);
text(0.1,tt-11*j,['num >= ' num2str(cos2) ' chip: ' num2str(sum(score_chip>=cos2))]);
print -djpeg mfold_known_bs_background

```

```

function mfe = anti_inds_to_mfe(anti_inds)
% anti_inds holds for each nuc in the seq what is the index of
% the nuc across from it where the 0 means unpaired (this is returned by read_structure_withanti).
% returns mfe which is the structure in the format of rnafold, i.e. only base pairs:
% mfe is a 2 col matrix, the first being the bases on arm5 which are paired and the second
% their corresponding pairs
if(~iscell(anti_inds))
    mfe = get_mfe(anti_inds);
    return;
end
for i=1:length(anti_inds)
    mfe{i} = get_mfe(anti_inds{i});
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function mfe = get_mfe(ai)
bps=0;
for i=1:length(ai)
    if(ai(i))
        if(i>ai(i))
            return
        end
        bps = bps+1;
        mfe(bps,1) = i;
        mfe(bps,2) = ai(i);
    end
end
mfold_cv_proto;
score(examples) = win_score(examples).*pos_score(examples);
%score(examples) = pos_score(examples);
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est(examples),score(examples),mirpos(examples),endbulges(examples));
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] =
analyse_errors_bins2(pos_est(examples),score(examples),mirpos(examples),endbulges(examples),num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
mfold_cv_proto;
%score(examples) = win_score(examples).*pos_score(examples);
score(examples) = win_score(examples);
%score(examples) = pos_score(examples);
for i=1:length(mirpos)
    mfe = mfes{i};
    pos_est_arm5(i) = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));

```

```

pos_est_arm3(i) = mfe(win_pos_est(i),2);
d5 = abs(pos_est_arm5(i)-mirpos(i));
d3 = abs(pos_est_arm3(i)-mirpos(i));
pos_error(i) = min(d5,d3);
if(d3<d5)
    pos_est_side_known(i) = pos_est_arm3(i);
else
    pos_est_side_known(i) = pos_est_arm5(i);
end
end
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est(examples),score(examples),mirpos(examples),endbulges(examples));
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] =
analyse_errors_bins2(pos_est(examples),score(examples),mirpos(examples),endbulges(examples),num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
figure
subplot(2,1,1)
res =
analyse_errors_perc(pos_est_side_known(examples),score(examples),mirpos(examples),endbulges(examples));
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] =
analyse_errors_bins2(pos_est_side_known(examples),score(examples),mirpos(examples),endbulges(examples),num
_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
save_mfold_data = 1;
filename = 'mfold_rand5_rundata.mat';
randstate=5;
mfold_cv_random;
%score = win_score.*pos_score;
score = win_score;
%score = pos_score;
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est,score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')

```

```

subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
if(save_mfold_data)
    eval(['save ' filename]);
end
mfold_cv_random;
%score = win_score.*pos_score;
score = win_score;
%score = pos_score;
for i=1:length(mirpos)
    mfe = mfes{i};
    pos_est_arm5(i) = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));
    pos_est_arm3(i) = mfe(win_pos_est(i),2);
    d5 = abs(pos_est_arm5(i)-mirpos(i));
    d3 = abs(pos_est_arm3(i)-mirpos(i));
    pos_error(i) = min(d5,d3);
    if(d3<d5)
        pos_est_side_known(i) = pos_est_arm3(i);
    else
        pos_est_side_known(i) = pos_est_arm5(i);
    end
end
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est,score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est_side_known,score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est_side_known,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;

```

```

legend('off')
mfold_cv_testwin_proto;
% chooses the correct side to only test win prediction and not side prediction
for i=1:length(examples)
    ind = examples(i);
    mfe = mfes{ind};
    pos_est_arm5 = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));
    pos_est_arm3 = mfe(win_pos_est(ind),2);
    d5 = abs(pos_est_arm5-mirpos(ind));
    d3 = abs(pos_est_arm3-mirpos(ind));
    pos_error(ind) = min(d5,d3);
    if(d3<d5)
        pos_est(ind) = pos_est_arm3;
    else
        pos_est(ind) = pos_est_arm5;
    end
end
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est(examples),win_score(examples),mirpos(examples),endbulges(examples));
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] =
analyse_errors_bins2(pos_est(examples),win_score(examples),mirpos(examples),endbulges(examples),num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
mfold_cv_testwin_random;
% chooses the correct side to only test win prediction and not side prediction
for i=1:length(mirpos)
    mfe = mfes{i};
    pos_est_arm5 = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));
    pos_est_arm3 = mfe(win_pos_est(i),2);
    d5 = abs(pos_est_arm5-mirpos(i));
    d3 = abs(pos_est_arm3-mirpos(i));
    pos_error(i) = min(d5,d3);
    if(d3<d5)
        pos_est(i) = pos_est_arm3;
    else
        pos_est(i) = pos_est_arm5;
    end
end
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est,win_score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')

```

```

subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,yp2,yp2] = analyse_errors_bins2(pos_est,win_score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
function model = bayes_learn_pos_given_win(seqs,anti_inds,bulges1,bulges2,endbulges,pos,mirlen,model)
%model is a struct.
% mfes{i} holds the structure in the basepair notation
mfes = anti_inds_to_mfe(anti_inds);
% win_pos(i) is the position of the window corresponding to mir i
win_pos = get_win_pos_v1(mfes,anti_inds,pos,mirlen);
possible_positions = get_possible_positions(model,mfes,endbulges,win_pos);
% for each seq hold the mirposition and all possible positions that are not mirpos
for i=1:length(pos)
    mirpos(i) = pos(i);
    nonmirpos{i} = setdiff(possible_positions{i},mirpos(i));
end
[upper_mean_dist,upper_std_dist,lower_mean_dist,lower_std_dist] = loopdist_model(mirpos,endbulges);
model.pos_upper_mean_dist = upper_mean_dist;
model.pos_upper_std_dist = upper_std_dist;
model.pos_lower_mean_dist = lower_mean_dist;
model.pos_lower_std_dist = lower_std_dist;
[p1_nuc_mir,p2_nuc_mir]= nucleotide_pos_model_list(model,seqs,mirpos);
[p1_nuc_nonmir,p2_nuc_nonmir]= nucleotide_pos_model_list(model,seqs,nonmirpos);
model.pos_p1_nuc_mir = p1_nuc_mir;
model.pos_p2_nuc_mir = p2_nuc_mir;
model.pos_p1_nuc_nonmir = p1_nuc_nonmir;
model.pos_p2_nuc_nonmir = p2_nuc_nonmir;
[pb1_mir,pb2_mir,pbtot_mir] = pos_bulge_pos_model_list(model,bulges1,bulges2,mirpos);
[pb1_nonmir,pb2_nonmir,pbtot_nonmir] = pos_bulge_pos_model_list(model,bulges1,bulges2,nonmirpos);
model.pos_pb1_mir = pb1_mir;
model.pos_pb1_nonmir = pb1_nonmir;
model.pos_pb2_mir = pb2_mir;
model.pos_pb2_nonmir = pb2_nonmir;
model.pos_pbtot_mir = pbtot_mir;
model.pos_pbtot_nonmir = pbtot_nonmir;
p_bp_mir = pos_base_pair_model_list(model,seqs,anti_inds,mirpos);
p_bp_nonmir = pos_base_pair_model_list(model,seqs,anti_inds,nonmirpos);
model.p_bp_mir = p_bp_mir;
model.p_bp_nonmir = p_bp_nonmir;
function model = bayes_learn_win(seqs,anti_inds,bulges1,bulges2,endbulges,pos,mirlen,model)
%model_params is a struct.
% mfes{i} holds the structure in the basepair notation
mfes = anti_inds_to_mfe(anti_inds);
% win_pos(i) is the position of the window corresponding to mir i
win_pos = get_win_pos_v1(mfes,anti_inds,pos,mirlen);
% for each seq hold the mirposition and all possible positions that are not mirpos
for i=1:length(pos)

```



```

mirwin(i) = win_pos(i);
n_bps = size(mfes{i},1);
nonmirwin{i} = setdiff([model.min_win_bp:n_bps],mirwin(i));
end
[mean_loopdist,std_loopdist] = loopdist_bp_model_normal(win_pos,mfes);
model.mean_loopdist_bp = mean_loopdist;
model.std_loopdist_bp = std_loopdist;
[win_num_bps_mir_vals,win_num_bps_mir_ps] = num_bps_model_hist_list(mfes,anti_inds,model,mirwin);
[win_num_bps_nonmir_vals,win_num_bps_nonmir_ps] = num_bps_model_hist_list(mfes,anti_inds,model,nonmirwin);
model.win_num_bps_mir_vals = win_num_bps_mir_vals;
model.win_num_bps_mir_ps = win_num_bps_mir_ps;
model.win_num_bps_nonmir_vals = win_num_bps_nonmir_vals;
model.win_num_bps_nonmir_ps = win_num_bps_nonmir_ps;
[win_sym_mir_vals,win_sym_mir_ps] = win_sym_model_list(mfes,anti_inds,model,mirwin);
[win_sym_nonmir_vals,win_sym_nonmir_ps] = win_sym_model_list(mfes,anti_inds,model,nonmirwin);
model.win_sym_mir_vals = win_sym_mir_vals;
model.win_sym_mir_ps = win_sym_mir_ps;
model.win_sym_nonmir_vals = win_sym_nonmir_vals;
model.win_sym_nonmir_ps = win_sym_nonmir_ps;
[pb_arm5_mir,pb_arm3_mir,pb1_arm5_mir,pb1_arm3_mir,pb2_arm5_mir,pb2_arm3_mir]...
    = win_bulge_pos_model_list(mfes,bulges1,bulges2,model,mirwin);
[pb_arm5_nonmir,pb_arm3_nonmir,pb1_arm5_nonmir,pb1_arm3_nonmir,pb2_arm5_nonmir,pb2_arm3_nonmir]...
    = win_bulge_pos_model_list(mfes,bulges1,bulges2,model,nonmirwin);
model.win_bulge_posit_arm5_mir = pb_arm5_mir;
model.win_bulge_posit_arm3_mir = pb_arm3_mir;
model.win_bulge1_posit_arm5_mir = pb1_arm5_mir;
model.win_bulge1_posit_arm3_mir = pb1_arm3_mir;
model.win_bulge2_posit_arm5_mir = pb2_arm5_mir;
model.win_bulge2_posit_arm3_mir = pb2_arm3_mir;
model.win_bulge_posit_arm5_nonmir = pb_arm5_nonmir;
model.win_bulge_posit_arm3_nonmir = pb_arm3_nonmir;
model.win_bulge1_posit_arm5_nonmir = pb1_arm5_nonmir;
model.win_bulge1_posit_arm3_nonmir = pb1_arm3_nonmir;
model.win_bulge2_posit_arm5_nonmir = pb2_arm5_nonmir;
model.win_bulge2_posit_arm3_nonmir = pb2_arm3_nonmir;
[win_p_bp_arm5_mir,win_p_bp_arm3_mir] = ...
    win_base_pair_model_list(mfes,anti_inds,seqs,model,mirwin);
[win_p_bp_arm5_nonmir,win_p_bp_arm3_nonmir] = ...
    win_base_pair_model_list(mfes,anti_inds,seqs,model,nonmirwin);
model.win_base_pair_arm5_mir = win_p_bp_arm5_mir;
model.win_base_pair_arm3_mir = win_p_bp_arm3_mir;
model.win_base_pair_arm5_nonmir = win_p_bp_arm5_nonmir;
model.win_base_pair_arm3_nonmir = win_p_bp_arm3_nonmir;
[p1_5_mir,p2_5_mir,p1_3_mir,p2_3_mir] = win_nuc_positional_model_list(seqs,mfes,model,mirwin);
[p1_5_nonmir,p2_5_nonmir,p1_3_nonmir,p2_3_nonmir] = ...
    win_nuc_positional_model_list(seqs,mfes,model,nonmirwin);
model.win_nuc_pos_p1_5_mir = p1_5_mir;
model.win_nuc_pos_p2_5_mir = p2_5_mir;
model.win_nuc_pos_p1_3_mir = p1_3_mir;
model.win_nuc_pos_p2_3_mir = p2_3_mir;

```

```

model.win_nuc_pos_p1_5_nonmir = p1_5_nonmir;
model.win_nuc_pos_p2_5_nonmir = p2_5_nonmir;
model.win_nuc_pos_p1_3_nonmir = p1_3_nonmir;
model.win_nuc_pos_p2_3_nonmir = p2_3_nonmir;
return
function [pos,score] = bayes_predict_pos_given_win(seqs,win_pos,anti_inds,bulges1,bulges2,endbulges,model)
mfes = anti_inds_to_mfe(anti_inds);
for i = 1:length(seqs)
    %disp(num2str(i));
    [posi, scorei] =
bayes_predict_side_i(model,seqs{i},win_pos(i),mfes{i},anti_inds{i},bulges1{i},bulges2{i},endbulges{i});
    pos(i) = posi;
    score(i) = scorei;
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [posi, scorei] = bayes_predict_side_i(model,seqsi,wp,mfei,ai,bulges1i,bulges2i,endbulgesi)
pl = get_possible_positions(model,mfei,endbulgesi,wp);
pos_list = pl{1};
p_loopdist = loopdist_prob(pos_list,model,endbulgesi);
[p_pos_nuc_mir,p_pos_nuc_nonmir] = nuc_pos_prob(pos_list,model,seqsi);
[p_pos_bulge_mir,p_pos_bulge_nonmir] = bulge_pos_prob(pos_list,model,bulges1i,bulges2i);
[p_base_pair_mir,p_base_pair_nonmir] = base_pair_prob(pos_list,model,seqsi,ai);
p_mir = ones(size(pos_list));
p_nonmir = ones(size(pos_list));
if(model.pos_use_loopdist)
    p_mir = p_mir.*p_loopdist;
    p_nonmir = p_nonmir.*(1-p_loopdist);
end
if(model.pos_use_pos_nuc)
    p_mir = p_mir.*p_pos_nuc_mir;
    p_nonmir = p_nonmir.*p_pos_nuc_nonmir;
end
if(model.pos_use_pos_bulge)
    p_mir = p_mir.*p_pos_bulge_mir;
    p_nonmir = p_nonmir.*p_pos_bulge_nonmir;
end
if(model.pos_use_base_pair)
    p_mir = p_mir.*p_base_pair_mir;
    p_nonmir = p_nonmir.*p_base_pair_nonmir;
end
I = find((p_mir + p_nonmir) > 0);
p(I) = p_mir(I)./(p_mir(I)+p_nonmir(I));
[scorei,pos_ind] = max(p);
posi = pos_list(pos_ind);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function p_loopdist = loopdist_prob(pos_list, model, endbulgesi);
% calculates the probability of each position in the list based on distance from loop

```

```

%uses gaussian probability distribution
seq_size = length(endbulgesi);
lb = find(endbulgesi);
eb_begin = lb(1);
eb_end = lb(end);
zloopdist = zeros(size(pos_list)); %standardized variables
side = sign(pos_list - eb_begin);
lup = find(side == -1);
zloopdist(lup) = (eb_begin - pos_list(lup) - model.pos_upper_mean_dist)/model.pos_upper_std_dist;
llw = find(side == 1);
zloopdist(llw) = (pos_list(llw)-eb_end - model.pos_lower_mean_dist)/model.pos_lower_std_dist;
p_loopdist = exp(-0.5*zloopdist.^2);
p_loopdist = p_loopdist/sum(p_loopdist);
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_nuc_mir,p_nuc_nonmir] = nuc_pos_prob(pos_list,model,seqsi);
p1_nuc_mir = model.pos_p1_nuc_mir;
p2_nuc_mir = model.pos_p2_nuc_mir;
p1_nuc_nonmir = model.pos_p1_nuc_nonmir;
p2_nuc_nonmir = model.pos_p2_nuc_nonmir;
win_len = model.win_len;
p_nuc_mir = zeros(size(pos_list));
p_nuc_nonmir = zeros(size(pos_list));
for i=1:length(pos_list)
    pos = pos_list(i);
    win_inds = pos:min([pos+win_len-1,length(seqsi)]);
    win_len_actual = length(win_inds);
    winseq = seqsi(win_inds);

    %multiply probabilities of single nucleotides in window 'win'
    if model.pos_nuc_order == 1
        %1 gram
        p_nuc_i = 1;
        for j = 1:win_len_actual
            p_nuc_i = p_nuc_i * p1_nuc_mir(j,winseq(j));
        end
    else
        %2 gram
        p_nuc_i = p1_nuc_mir(1,winseq(1));
        for j = 1:win_len_actual-1
            p_nuc_i = p_nuc_i * ...
                p2_nuc_mir(j,winseq(j),winseq(j+1))/p1_nuc_mir(j,winseq(j));
        end
    end
    %normalize by window length
    p_nuc_mir(i) = p_nuc_i^(win_len/win_len_actual);
    %calculate p(win given nonmir)
    if model.pos_nuc_order == 1
        p_nuc_i = 1;

```

```

for j = 1:win_len_actual
    p_nuc_i = p_nuc_i * p1_nuc_nonmir(winseq(j));
end
else
    p_nuc_i = p1_nuc_nonmir(1,winseq(1));
for j = 1:win_len_actual-1
    p_nuc_i = p_nuc_i * p2_nuc_nonmir(j,winseq(j),winseq(j+1))/p1_nuc_nonmir(j,winseq(j));
end
end
%normalize by window length
p_nuc_nonmir(i) = p_nuc_i^(win_len/win_len_actual);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_bulge_mir,p_bulge_nonmir] = bulge_pos_prob(pos_list,model,bulges1i,bulges2i);
win_len = model.win_len;
if(model.pos_bulge == 1)
    pb_mir = model.pos_pb1_mir;
    pb_nonmir = model.pos_pb1_nonmir;
    bulges = bulges1i;
elseif(model.pos_bulge == 2)
    pb_mir = model.pos_pb2_mir;
    pb_nonmir = model.pos_pb2_nonmir;
    bulges = bulges2i;
elseif(model.pos_bulge == 0)
    pb_mir = model.pos_pbtot_mir;
    pb_nonmir = model.pos_pbtot_nonmir;
    bulges = bulges1i+bulges2i;
else
    error('model.pos_bulge must be 1 2 or 0');
end
p_bulge_mir = zeros(size(pos_list));
p_bulge_nonmir = zeros(size(pos_list));
for i=1:length(pos_list)
    pos = pos_list(i);
    win_inds = pos:min([pos+win_len-1,length(bulges)]);
    win_len_actual = length(win_inds);
    winbulges = bulges(win_inds);
    J0 = find(winbulges == 0);
    J1 = find(winbulges);
    p_bulge_i = prod(pb_mir(J1)) * prod(1-pb_mir(J0));
    p_bulge_mir(i) = p_bulge_i^(win_len/win_len_actual);
    p_bulge_i = prod(pb_nonmir(J1)) * prod(1-pb_nonmir(J0));
    p_bulge_nonmir(i) = p_bulge_i^(win_len/win_len_actual);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_base_pair_mir,p_base_pair_nonmir] = base_pair_prob(pos_list,model,seqsi,ai);
win_len = model.win_len;
p_bp_mir = model.p_bp_mir;

```

```

p_bp_nonmir = model.p_bp_nonmir;
seqbp = nuc2bp(seqsi,ai,model.pos_base_pair_states);
p_base_pair_mir = zeros(size(pos_list));
p_base_pair_nonmir = zeros(size(pos_list));
for i=1:length(pos_list)
    pos = pos_list(i);
    win_inds = pos:min([pos+win_len-1,length(seqsi)]);
    win_len_actual = length(win_inds);
    pmir_i = 1;
    pnonmir_i = 1;
    for j = 1:model.pos_base_pair_states
        pmir_i = pmir_i * p_bp_mir(j)^sum(seqbp(win_inds) == j);
        pnonmir_i = pnonmir_i * p_bp_nonmir(j)^sum(seqbp(win_inds) == j);
    end
    p_base_pair_mir(i) = pmir_i^(win_len/win_len_actual);
    p_base_pair_nonmir(i) = pnonmir_i^(win_len/win_len_actual);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [win_pos,win_score] = bayes_predict_win(model,seqs,anti_inds,bulges1,bulges2,endbulges)
%[win_pos,score] = bayes_predict_win(model,seqs,anti_inds,bulges1,bulges2,endbulges)
% find the best window position by its matching to the bayesian model
mfes = anti_inds_to_mfe(anti_inds);
for i = 1:length(seqs)
    %disp(num2str(i));
    [win_posi, win_scorei] = bayes_predict_win_i(model,seqs{i},mfes{i},anti_inds{i},bulges1{i},bulges2{i},endbulges{i});
    win_pos(i) = win_posi;
    win_score(i) = win_scorei;
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [win_pos, win_score] = bayes_predict_win_i(model,seqsi,mfei,ai,bulges1i,bulges2i, endbulgesi);
p_loopdist = loopdist_bp_prob_normal(model,mfei);
[p_num_bps_mir,p_num_bps_nonmir] = num_bps_prob_hist(model,mfei,ai);
[p_win_sym_mir,p_win_sym_nonmir] = win_sym_prob(model,mfei,ai);
[p_pos_bulge_mir,p_pos_bulge_nonmir] = win_bulges_pos_prob(model,mfei,bulges1i,bulges2i,0);
[p_base_pair_mir,p_base_pair_nonmir] = win_base_pair_prob(model,mfei,ai,seqsi);
[p_nuc_mir,p_nuc_nonmir] = win_nuc_positional_prob_sw(model,seqsi,mfei);
p_mir = ones(1,size(mfei,1));
p_nonmir = ones(1,size(mfei,1));
if(model.win_use_loopdist)
    p_mir = p_mir.*p_loopdist;
    p_nonmir = p_nonmir.*(1-p_loopdist);
end
if(model.win_use_num_bps)
    p_mir = p_mir.*p_num_bps_mir;
    p_nonmir = p_nonmir.*p_num_bps_nonmir;
end
if(model.win_use_win_sym)

```

```

    p_mir = p_mir.*p_win_sym_mir;
    p_nonmir = p_nonmir.*p_win_sym_nonmir;
end
if(model.win_use_pos_bulge)
    p_mir = p_mir.*p_pos_bulge_mir;
    p_nonmir = p_nonmir.*p_pos_bulge_nonmir;
end
if(model.win_use_base_pair)
    p_mir = p_mir.*p_base_pair_mir;
    p_nonmir = p_nonmir.*p_base_pair_nonmir;
end
if(model.win_use_nuc)
    p_mir = p_mir.*p_nuc_mir;
    p_nonmir = p_nonmir.*p_nuc_nonmir;
end
I = find((p_mir + p_nonmir) > 0);
p(I) = p_mir(I)./(p_mir(I)+p_nonmir(I));
[win_score,win_pos] = max(p);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function p_loopdist = loopdist_bp_prob_normal(model,mfe);
n_bps = size(mfe,1);
wp = 1:n_bps;
zloopdist = ((n_bps - wp) - model.mean_loopdist_bp)/model.std_loopdist_bp;
zloopdist(1:model.min_win_bp-1) = 0; % illegal windows.
p_loopdist = exp(-0.5*zloopdist.^2);
p_loopdist = p_loopdist/sum(p_loopdist);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_num_bps_mir,p_num_bps_nonmir] = num_bps_prob_hist(model,mfe,ai);
win_len = model.win_len;
n_bps = size(mfe,1);
p_num_bps_mir = zeros(1,n_bps);
p_num_bps_nonmir = zeros(1,n_bps);
is_paired = (ai~=0);
for wp = model.min_win_bp:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
    win5inds = pos5_on_arm5:pos3_on_arm5;
    win3inds = pos5_on_arm3:pos3_on_arm3;
    numpaired5 = sum(is_paired(win5inds));
    numpaired3 = sum(is_paired(win3inds));
    num_bps_i = min(numpaired5,numpaired3);
    % mir
    tt = find(model.win_num_bps_mir_vals == num_bps_i);
    if(tt)
        p_num_bps_mir_i = model.win_num_bps_mir_ps(tt);
    else

```

```

    p_num_bps_mir_i = 0;
end
p_num_bps_mir_i = p_num_bps_mir_i*(win_len/mean(length(win5inds),length(win3inds)));
p_num_bps_mir(wp) = p_num_bps_mir_i;
% nonmir
tt = find(model.win_num_bps_nonmir_vals == num_bps_i);
if(tt)
    p_num_bps_nonmir_i = model.win_num_bps_nonmir_ps(tt);
else
    p_num_bps_nonmir_i = 0;
end
p_num_bps_nonmir_i = p_num_bps_nonmir_i*(win_len/mean(length(win5inds),length(win3inds)));
p_num_bps_nonmir(wp) = p_num_bps_nonmir_i;
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_win_sym_mir,p_win_sym_nonmir] = win_sym_prob(model,mfe,ai);
win_len = model.win_len;
n_bps = size(mfe,1);
p_win_sym_mir = zeros(1,n_bps);
p_win_sym_nonmir = zeros(1,n_bps);
is_paired = (ai~=0);
for wp = model.min_win_bp:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
    win5inds = pos5_on_arm5:pos3_on_arm5;
    win3inds = pos5_on_arm3:pos3_on_arm3;
    numunpaired5 = sum(~is_paired(win5inds));
    numunpaired3 = sum(~is_paired(win3inds));
    win_sym_i = abs(numunpaired5-numunpaired3);
    % mir
    tt = find(model.win_sym_mir_vals == win_sym_i);
    if(tt)
        p_win_sym_mir_i = model.win_sym_mir_ps(tt);
    else
        p_win_sym_mir_i = 0;
    end
    p_win_sym_mir_i = p_win_sym_mir_i*sqrt(win_len/mean(length(win5inds),length(win3inds)));
    p_win_sym_mir(wp) = p_win_sym_mir_i;
    % nonmir
    tt = find(model.win_sym_nonmir_vals == win_sym_i);
    if(tt)
        p_win_sym_nonmir_i = model.win_sym_nonmir_ps(tt);
    else
        p_win_sym_nonmir_i = 0;
    end
    p_win_sym_nonmir_i = p_win_sym_nonmir_i*sqrt(win_len/mean(length(win5inds),length(win3inds)));
    p_win_sym_nonmir(wp) = p_win_sym_nonmir_i;
end

```

```

end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_pos_bulge_mir,p_pos_bulge_nonmir] = win_bulges_pos_prob(model,mfe,bulges1i,bulges2i,use_avg);
bulge_flag = model.win_bulge;
win_len = model.win_len;
n_bps = size(mfe,1);
p_pos_bulge_mir = zeros(1,n_bps);
p_pos_bulge_nonmir = zeros(1,n_bps);
pb_arm5_mir = model.win_bulge_posit_arm5_mir;
pb_arm3_mir = model.win_bulge_posit_arm3_mir;
pb1_arm5_mir = model.win_bulge1_posit_arm5_mir;
pb1_arm3_mir = model.win_bulge1_posit_arm3_mir;
pb2_arm5_mir = model.win_bulge2_posit_arm5_mir;
pb2_arm3_mir = model.win_bulge2_posit_arm3_mir;
pb_arm5_nonmir = model.win_bulge_posit_arm5_nonmir;
pb_arm3_nonmir = model.win_bulge_posit_arm3_nonmir;
pb1_arm5_nonmir = model.win_bulge1_posit_arm5_nonmir;
pb1_arm3_nonmir = model.win_bulge1_posit_arm3_nonmir;
pb2_arm5_nonmir = model.win_bulge2_posit_arm5_nonmir;
pb2_arm3_nonmir = model.win_bulge2_posit_arm3_nonmir;
if(use_avg)
    pb_mir = 0.5*(pb_arm5_mir+pb_arm3_mir);
    pb_arm5_mir = pb_mir;
    pb_arm3_mir = pb_mir;
    pb1_mir = 0.5*(pb1_arm5_mir+pb1_arm3_mir);
    pb1_arm5_mir = pb1_mir;
    pb1_arm3_mir = pb1_mir;
    pb2_mir = 0.5*(pb2_arm5_mir+pb2_arm3_mir);
    pb2_arm5_mir = pb2_mir;
    pb2_arm3_mir = pb2_mir;
    pb_nonmir = 0.5*(pb_arm5_nonmir+pb_arm3_nonmir);
    pb_arm5_nonmir = pb_nonmir;
    pb_arm3_nonmir = pb_nonmir;
    pb1_nonmir = 0.5*(pb1_arm5_nonmir+pb1_arm3_nonmir);
    pb1_arm5_nonmir = pb1_nonmir;
    pb1_arm3_nonmir = pb1_nonmir;
    pb2_nonmir = 0.5*(pb2_arm5_nonmir+pb2_arm3_nonmir);
    pb2_arm5_nonmir = pb2_nonmir;
    pb2_arm3_nonmir = pb2_nonmir;
end
if(bulge_flag == 1)
    pb_arm5_mir = pb1_arm5_mir;
    pb_arm3_mir = pb1_arm3_mir;
    pb_arm5_nonmir = pb1_arm5_nonmir;
    pb_arm3_nonmir = pb1_arm3_nonmir;
    bulgesi = bulges1i;
elseif(bulge_flag == 2)
    pb_arm5_mir = pb2_arm5_mir;
    pb_arm3_mir = pb2_arm3_mir;

```



```

pb_arm5_nonmir = pb2_arm5_nonmir;
pb_arm3_nonmir = pb2_arm3_nonmir;
bulgesi = bulges2i;
else
    % just use the total pb.
    bulgesi = bulges1i+bulges2i;
end
for wp = model.min_win_bp:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(bulgesi),pos5_on_arm3+win_len-1);
    win5 = bulgesi(pos3_on_arm5:-1:pos5_on_arm5); % always start from loop side
    win3 = bulgesi(pos5_on_arm3:pos3_on_arm3);
    win5_len_actual = length(win5);
    win3_len_actual = length(win3);

    J0 = find(win5 == 0);
    J1 = find(win5);
    p_bulges5_mir_i = prod(pb_arm5_mir(J1)) * prod(1-pb_arm5_mir(J0));
    p_bulges5_mir_i = p_bulges5_mir_i^(win_len/win5_len_actual);
    p_bulges5_nonmir_i = prod(pb_arm5_nonmir(J1)) * prod(1-pb_arm5_nonmir(J0));
    p_bulges5_nonmir_i = p_bulges5_nonmir_i^(win_len/win5_len_actual);
    J0 = find(win3 == 0);
    J1 = find(win3);
    p_bulges3_mir_i = prod(pb_arm3_mir(J1)) * prod(1-pb_arm3_mir(J0));
    p_bulges3_mir_i = p_bulges3_mir_i^(win_len/win3_len_actual);
    p_bulges3_nonmir_i = prod(pb_arm3_nonmir(J1)) * prod(1-pb_arm3_nonmir(J0));
    p_bulges3_nonmir_i = p_bulges3_nonmir_i^(win_len/win3_len_actual);

    p_pos_bulge_mir(wp) = sqrt(p_bulges5_mir_i*p_bulges3_mir_i);
    p_pos_bulge_nonmir(wp) = sqrt(p_bulges5_nonmir_i*p_bulges3_nonmir_i);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_base_pair_mir,p_base_pair_nonmir] = win_base_pair_prob(model,mfe,ai,seq);
win_len = model.win_len;
base_pair_states = model.win_base_pair_states;
p_bp_arm5_mir = model.win_base_pair_arm5_mir;
p_bp_arm3_mir = model.win_base_pair_arm3_mir;
p_bp_arm5_nonmir = model.win_base_pair_arm5_nonmir;
p_bp_arm3_nonmir = model.win_base_pair_arm3_nonmir;
n_bps = size(mfe,1);
p_base_pair = zeros(1,n_bps);
t1{1} = seq;
t2{1} = ai;
t3 = nuc2bp(t1,t2,base_pair_states);
seqbp = t3{1};
for wp = model.min_win_bp:n_bps
    pos3_on_arm5 = mfe(wp,1);

```

```

pos5_on_arm3 = mfe(wp,2);
pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
win5inds = (pos5_on_arm5:pos3_on_arm5);
win3inds = (pos5_on_arm3:pos3_on_arm3);
% mir
p5_mir_i = 1;
p3_mir_i = 1;
for j = 1:base_pair_states
    p5_mir_i = p5_mir_i * p_bp_arm5_mir(j)^sum(seqbp(win5inds) == j);
    p3_mir_i = p3_mir_i * p_bp_arm3_mir(j)^sum(seqbp(win3inds) == j);
end
p5_mir_i = p5_mir_i.^(win_len/length(win5inds));
p3_mir_i = p3_mir_i.^(win_len/length(win3inds));
p_base_pair_mir(wp) = sqrt(p5_mir_i*p3_mir_i);
% nonmir
p5_nonmir_i = 1;
p3_nonmir_i = 1;
for j = 1:base_pair_states
    p5_nonmir_i = p5_nonmir_i * p_bp_arm5_nonmir(j)^sum(seqbp(win5inds) == j);
    p3_nonmir_i = p3_nonmir_i * p_bp_arm3_nonmir(j)^sum(seqbp(win3inds) == j);
end
p5_nonmir_i = p5_nonmir_i.^(win_len/length(win5inds));
p3_nonmir_i = p3_nonmir_i.^(win_len/length(win3inds));
p_base_pair_nonmir(wp) = sqrt(p5_nonmir_i*p3_nonmir_i);
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_nuc_mir,p_nuc_nonmir] = win_nuc_positional_prob_sw(model,seq,mfe);
% look at AT as one thing and at CG as one
% for now implemented only 1gram of this version
win_len = model.win_len;
win_len_common = min(win_len,model.win_nuc_pos_win);
p1_5_mir = model.win_nuc_pos_p1_5_mir;
p2_5_mir = model.win_nuc_pos_p2_5_mir;
p1_3_mir = model.win_nuc_pos_p1_3_mir;
p2_3_mir = model.win_nuc_pos_p2_3_mir;
p1_5_nonmir = model.win_nuc_pos_p1_5_nonmir;
p2_5_nonmir = model.win_nuc_pos_p2_5_nonmir;
p1_3_nonmir = model.win_nuc_pos_p1_3_nonmir;
p2_3_nonmir = model.win_nuc_pos_p2_3_nonmir;
p1_5_mir = transform_p1(p1_5_mir);
p1_3_mir = transform_p1(p1_3_mir);
p1_5_nonmir = transform_p1(p1_5_nonmir);
p1_3_nonmir = transform_p1(p1_3_nonmir);
p2_5_mir = transform_p2(p2_5_mir);
p2_3_mir = transform_p2(p2_3_mir);
p2_5_nonmir = transform_p2(p2_5_nonmir);
p2_3_nonmir = transform_p2(p2_3_nonmir);
n_bps = size(mfe,1);

```

```

for wp = model.min_win_bp:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(seq),pos5_on_arm3+win_len-1);
    win5inds = (pos5_on_arm5:pos3_on_arm5);
    win3inds = (pos5_on_arm3:pos3_on_arm3);

    seq5_sw = transform_to_sw(seq(win5inds));
    seq3_sw = transform_to_sw(seq(win3inds));

    win5_len_actual = min(model.win_nuc_pos_win,length(seq5_sw));
    win3_len_actual = min(model.win_nuc_pos_win,length(seq3_sw));

    % mir
    if model.win_nuc_order == 1
        %1 gram
        p5_i = 1;
        for j = 1:win5_len_actual
            p5_i = p5_i * p1_5_mir(j,seq5_sw(j));
        end
        p3_i = 1;
        for j = 1:win3_len_actual
            p3_i = p3_i * p1_3_mir(j,seq3_sw(j));
        end
    else
        %2 gram
        p5_i = p1_5_mir(1,seq5_sw(1));
        for j = 1:win5_len_actual-1
            p5_i = p5_i * p2_5_mir(j,seq5_sw(j),seq5_sw(j+1))/p1_5_mir(j,seq5_sw(j));
        end
        p3_i = p1_3_mir(1,seq3_sw(1));
        for j = 1:win3_len_actual-1
            p3_i = p3_i * p2_3_mir(j,seq3_sw(j),seq3_sw(j+1))/p1_3_mir(j,seq3_sw(j));
        end
    end
    p5_i = p5_i.^(win_len_common/win5_len_actual);
    p3_i = p3_i.^(win_len_common/win3_len_actual);
    p_nuc_mir(wp) = sqrt(p5_i*p3_i);

    % nonmir
    if model.win_nuc_order == 1
        %1 gram
        p5_i = 1;
        for j = 1:win5_len_actual
            p5_i = p5_i * p1_5_nonmir(j,seq5_sw(j));
        end
        p3_i = 1;
        for j = 1:win3_len_actual
            p3_i = p3_i * p1_3_nonmir(j,seq3_sw(j));
        end
    end

```

```

    end
else
    %2 gram
    p5_i = p1_5_nonmir(1,seq5_sw(1));
    for j = 1:win5_len_actual-1
        p5_i = p5_i * p2_5_nonmir(j,seq5_sw(j),seq5_sw(j+1))/p1_5_nonmir(j,seq5_sw(j));
    end
    p3_i = p1_3_nonmir(1,seq3_sw(1));
    for j = 1:win3_len_actual-1
        p3_i = p3_i * p2_3_nonmir(j,seq3_sw(j),seq3_sw(j+1))/p1_3_nonmir(j,seq3_sw(j));
    end
end
end
p5_i = p5_i.^(win_len_common/win5_len_actual);
p3_i = p3_i.^(win_len_common/win3_len_actual);
p_nuc_nonmir(wp) = sqrt(p5_i*p3_i);
end
function s = transform_to_sw(seq)
for i=1:length(seq)
    if(seq(i)==1 | seq(i)==3)
        s(i)=1;
    else
        s(i)=2;
    end
end
end
function p1 = transform_p1(p1_in)
p1_new(1,:) = mean([p1_in(:,1),p1_in(:,3)]');
p1_new(2,:) = mean([p1_in(:,2),p1_in(:,4)]');
p1 = p1_new';
function p2 = transform_p2(p2_in)
Ns = size(p2_in,2);
for j=1:size(p2_in,1)
    tt = reshape(p2_in(j,:,:),Ns,Ns);
    ttt(:,1) = (mean([tt(:,1),tt(:,3)]'))';
    ttt(:,2) = (mean([tt(:,2),tt(:,4)]'))';
    tttt(1,:) = mean([ttt(1,:);ttt(3,:)]);
    tttt(2,:) = mean([ttt(2,:);ttt(4,:)]);
    p2_new(j,:,:) = tttt;
end
end
p2 = p2_new;
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function positions = get_possible_positions(model,mfes,endbulges,win_pos)
% function positions = get_possible_positions(model,mfes,endbulges,win_pos)
% positions{i} a list of possible positions given the window position win_pos(i)
% for each arm gives pos5 of the window on that arm plus model.possible_pos_back
% positions back and model.possible_pos_fwd positions fwd.
% will also work with win_pos of length=1 and endbulges being a vector instead of a cell
win_len = model.win_len;
naway = model.possible_pos_away;
nto = model.possible_pos_to;

```

```

if(naway<0 | nto<0)
    error('model.possible_pos_away and model.possible_pos_to must be nonnegative')
end
if(length(win_pos)==1)
    tt{1} = endbulges;
    endbulges = tt;
    ttt{1} = mfes;
    mfes = ttt;
end
for i=1:length(win_pos)
    wp = win_pos(i);
    endbulgesi = endbulges{i};
    mfe = mfes{i};
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);

    t5 = [max(1,pos5_on_arm5-naway) : pos5_on_arm5+nto];
    t3 = [pos5_on_arm3-nto : min(length(endbulgesi),pos5_on_arm3+naway)];
    % remove indices sitting on end bulge
    lb = find(endbulgesi);
    positions{i} = setdiff([t5,t3],lb);
end
function win_mirpos = get_win_pos_v1(mfes,anti_inds,mirpos,mirlen)
% function win_mirpos = get_win_pos(mfes,anti_inds,mirpos,mirlen)
% returns win_mirpos in index of basepair (from legs not loop).
% i.e. mfe(win_mirpos,1) is the nuc pos on the 5 arm
% for mir on arm3 returns the closest bp from its mirpos towards the legs
% for mir on arm5 returns the closest bp from its END (mirpos+mirlen-1) towards the legs
% also towards the legs
for i=1:length(mirpos)
    pos5 = mirpos(i);
    pos3 = pos5+mirlen(i)-1;
    mfe = mfes{i};
    arm5 = mfe(:,1);
    arm3 = mfe(:,2);
    eb_start = arm5(end)+1;
    eb_end = arm3(end)-1;
    eb_len = eb_end-eb_start+1;
    side5 = (pos5<eb_start);
    ai = anti_inds{i};
    is_paired = (ai~=0);
    if(side5)
        k=0;
        while(~is_paired(pos3-k))
            k=k+1;
        end
        win_mirpos(i) = find(arm5==(pos3-k));
    else
        k=0;

```

```

while(~is_paired(pos5+k))
    k=k+1;
end
win_mirpos(i) = find(arm3==(pos5+k));
end
if isempty(win_mirpos(i))
    error('get_win_pos: fatal error. aborting.');
```

```

end
end
function strseq = int2nuc(intseq, ncase)
%strseq = int2nuc(intseq, ncase)
%convert a sequence of '1 2 3 4' into 'A C T G' or 'a c t g'
% ncase = uppercase | lowercase
if(isletter(intseq(1)))
    strseq = intseq;
    return;
end
if nargin == 1
    ncase = 'uppercase';
end
if strcmp(ncase,'uppercase')
    nucs = 'ACTG';
elseif strcmp(ncase,'lowercase')
    nucs = 'actg';
end
strseq = char(size(intseq));
for i = 1:length(intseq)
    strseq(i) = nucs(intseq(i));
end
return
function [yside, yprec2] = interpolate_prob_new(score, fitfile);
%[yside, yprec2] = interpolate_prob_new(score, fitfile);
% load the parameters for interpolation
load(fitfile);
%interpolate
yside = interp1(xs,ys,score,'linear');
yprec2 = interp1(xp2,yp2,score,'linear');
% extrapolate if necessary
if(min(xs)==xs(1)) % x is increasing
    yside(score<xs(1)) = ys(1);
    yprec2(score<xp2(1)) = yp2(1);
    yside(score>xs(end)) = ys(end);
    yprec2(score>xp2(end)) = yp2(end);
else % x is decreasing
    yside(score>xs(1)) = ys(1);
    yprec2(score>xp2(1)) = yp2(1);
    yside(score<xs(end)) = ys(end);
    yprec2(score<xp2(end)) = yp2(end);
end
returnfunction [mean_dist,std_dist] = loopdist_bp_model_normal(win_pos,mfes)

```

```

for i=1:length(win_pos)
    n_bps = size(mfes{i},1);
    loopdist(i) = n_bps - win_pos(i);
end
% cut off outliers
lp = prctile(loopdist,[2.5 97.5]);
I = find(loopdist >= lp(1) & loopdist <=lp(2));
mean_dist = mean(loopdist(I));
std_dist = std(loopdist(I));
%figure;hist(loopdist,[0:max(loopdist+1)]);title('loopdist training');function
[upper_mean_dist,upper_std_dist,lower_mean_dist,lower_std_dist] = loopdist_model(pos, endbulges)
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    side(i) = sign(pos(i) - eb(1)) ;
    loopdist(i) = 0.5* ( (1-side(i))*(eb(1) - pos(i)) + ...
        (1+side(i))*(pos(i)-eb(length(eb)))));
end
%keyboard
%upper strand
I = find(side == -1);
% cut off outliers
lp = prctile(loopdist(I),[2.5 97.5]);
I = find(side == -1 & loopdist > lp(1) & loopdist <lp(2));
upper_mean_dist = mean(loopdist(I));
upper_std_dist = std(loopdist(I));
%lower strand
I = find(side == 1);
% cut off outliers
lp = prctile(loopdist(I),[2.5 97.5]);
I = find(side == 1 & loopdist > lp(1) & loopdist <lp(2));
lower_mean_dist = mean(loopdist(I));
lower_std_dist = std(loopdist(I));
return
if(~exist('maxd'))
    maxd = 4;
end
randomize=0;
filename =['C:\rosetta\data_baseline_29_7\clust_proto_' num2str(maxd) '_' set_name '.txt'];
clust_proto = load(filename);
if length(clust_proto) ~= length(palseq)
    error('clust_proto wrong size');
end
if exist('randomize')
    if randomize == 1
        error('should load training set with randomize = 0 option');
    end
end
if(~exist('param_file'))
    params_tests;
else

```

```

    eval(param_file);
end
model = model_params;
mfes = anti_inds_to_mfe(anti_inds);
% win_pos(i) is the position of the window corresponding to mir i
win_pos = get_win_pos_v1(mfes,anti_inds,mirpos,mirlen);
n_all = length(palseq);
examples = find(clust_proto==1);
length(examples)
for i=1:length(examples)
    i
    bs = examples(i);% test set
    bt = setdiff(examples, bs);% train set

    model =
    bayes_learn_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt),mirpos(bt),mirlen(bt),model);
    model =
    bayes_learn_pos_given_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt),mirpos(bt),mirlen(bt),model);

    [win_pos_estm,win_scorem] =
    bayes_predict_win(model,palseq(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs));
    win_pos_est(bs) = win_pos_estm;
    win_score(bs) =win_scorem;

    % use estimated win_pos for prediction of pos!
    [pos_estm,pos_scorem]
    =bayes_predict_pos_given_win(palseq(bs),win_pos_est(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs),model);
    pos_est(bs) = pos_estm;
    pos_score(bs) = pos_scorem;
end
%modelrandomize=1;
if randomize
    rand('state',randstate);
    %rand('state',sum(100*clock));
    disp('performing randomized permutation');
    I = randperm(length(palseq));
    bulges1 = bulges1(I);
    bulges2 = bulges2(I);
    anti_inds = anti_inds(I);
    endbulges = endbulges(I);
    pal_id = pal_id(I);
    energy = energy(I);
    palseq = palseq(I);
    mirseq = mirseq(I);
    mirlen = mirlen(I);
    mirpos = mirpos(I);
    mfes = mfes(I);
end

```



```

if(~exist('mfold'))
    mfold = 3;
end
eval(param_file);
model = model_params;
n_all = length(palseq);
bins = round(0:n_all/mfold:n_all);
bins_all = 1:n_all;
m = 1;
while m <= mfold
    disp(num2str(m));

    bs = [bins(m)+1: bins(m+1)];% test set
    bt = setdiff(bins_all , bs);% train set

    disp(' ');
    disp(['m = ' num2str(m)]);

    model =
    bayes_learn_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt),mirpos(bt),mirlen(bt),model);
    model =
    bayes_learn_pos_given_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt),mirpos(bt),mirlen(bt),model);

    [win_pos_estm,win_scorem] =
    bayes_predict_win(model,palseq(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs));
    win_pos_est(bs) = win_pos_estm;
    win_score(bs) =win_scorem;

    % use estimated win_pos for prediction of pos!
    [pos_estm,pos_scorem]
    =bayes_predict_pos_given_win(palseq(bs),win_pos_est(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs),model);
    pos_est(bs) = pos_estm;
    pos_score(bs) = pos_scorem;

    m = m+1;
end
%modelmaxd = 4;
randomize=0;
filename =['C:\rosetta\data_baseline_29_7\clust_proto_' num2str(maxd) '_' set_name '.txt'];
clust_proto = load(filename);
if length(clust_proto) ~= length(palseq)
    error('clust_proto wrong size');
end
if exist('randomize')
    if randomize == 1
        error('should load training set with randomize = 0 option');
    end
end
end

```

```

if(~exist('param_file'))
    params_tests;
else
    eval(param_file);
end
model = model_params;
n_all = length(palseq);
examples = find(clust_proto==1);
length(examples)
for i=1:length(examples)
    bs = examples(i);% test set
    bt = setdiff(examples, bs);% train set

    model =
    bayes_learn_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt),mirpos(bt),mirlen(bt),model);
    [win_pos_estm,win_scorem] =
    bayes_predict_win(model,palseq(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs));

    win_pos_est(bs) = win_pos_estm;
    win_score(bs) =win_scorem;
end
modelrandomize=1;
if randomize
    rand('state',sum(100*clock));
    disp('performing randomized permutation');
    l = randperm(length(palseq));
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    anti_inds = anti_inds(l);
    endbulges = endbulges(l);
    pal_id = pal_id(l);
    energy = energy(l);
    palseq = palseq(l);
    mirseq = mirseq(l);
    mirlen = mirlen(l);
    mirpos = mirpos(l);
    mfes = mfes(l);
end
if(~exist('mfold'))
    mfold = 10;
end
if(~exist('param_file'))
    params_tests;
else
    eval(param_file);
end
model = model_params;
n_all = length(palseq);
bins = round(0:n_all/mfold:n_all);
bins_all = 1:n_all;

```

```

m = 1;
while m <= mfold
    disp(num2str(m));

    bs = [bins(m)+1: bins(m+1)];% test set
    bt = setdiff(bins_all , bs);% train set

    disp(' ');
    disp(['m = ' num2str(m)]);

    model =
    bayes_learn_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt),mirpos(bt),mirlen(bt),model);
    [win_pos_estm,win_scorem] =
    bayes_predict_win(model,palseq(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs));

    win_pos_est(bs) = win_pos_estm;
    win_score(bs) =win_scorem;

    m = m+1;
end
modelfunction seqsbp = nuc2bp(seqs,anti_inds,base_pair_basis)
%seqsbp = nuc2bp(seqs,anti_inds,base_pair_basis)
%transform to base pair representation
%for a 3 state model {AT,CG,TG} -> 1 2 3
%for a 6 state {AT,CG,TG,TA,GC,GT} -> 1 2 3 4 5 6
%also works if seqs is a vector and not a cell array, in which case returns a vector
if(~iscell(seqs))
    tt{1} = seqs;
    seqs = tt;
    tt{1} = anti_inds;
    anti_inds = tt;
    vecflag = 1;
else
    vecflag = 0;
end
map = zeros(4);
map(1,3) = 1; %AT
map(2,4) = 2; %CG
map(3,4) = 3; %TG
if base_pair_basis == 3
    map = map+map';
else
    map(3,1) = 4; %AT
    map(4,2) = 5; %CG
    map(4,3) = 6; %TG
end
seqsbp = cell(size(seqs));
for i = 1:length(seqs)
    seqsi = seqs{i};
    seqsbpi = zeros(size(seqsi));

```

```

anti_insi = anti_insi{i};

l = find(anti_insi ~= 0);
for j = 1:length(l)
    ij = l(j);
    seqsbpi(ij) = map(seqsi(ij),seqsi(anti_insi(ij)));
end
seqsbp{i} = seqsbpi;
end
if(vecflag)
    tt=seqsbp{1};
    seqsbp = tt;
end
return
function [intseq, fault_seq] = nuc2int4_new(strseq);
%[intseq, fault_seq] = nuc2int4_new(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
intseq = zeros(size(strseq));
fault_seq = 0;
for i = 1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i) = 1;
        case 'C' , intseq(i) = 2;
        case 'T' , intseq(i) = 3;
        case 'G' , intseq(i) = 4;
        otherwise , intseq = []; fault_seq = 1; break;
    end
end
end
function [p1,p2]= nucleotide_pos_model_list(model,seqs,positions);
% function [p1,p2]= nucleotide_pos_model_list(model,seqs,positions);
% learns a nucleotide positional model of a list of positions
% positions{i} is the list of positions on seqs{i}
% will work also if positions is a vector and not a cell
win_len = model.win_len;
numseqs = length(positions);
if(numseqs~=length(seqs))
    error('number of seqs differs from length(positions)');
end
% transform positions into cell if it is not so.
if(~iscell(positions))
    for i=1:numseqs
        tt{i} = positions(i);
    end
    positions = tt;
end
beta = 0.5;
Ns = 4; %number of states
c1 = zeros(win_len,Ns);
c2 = beta*ones(win_len-1,Ns,Ns);
p1 = c1;

```

```

p2 = c2;
for i = 1:numseqs
    seq = seqs{i};
    pos_list = positions{i};
    for k = 1:length(pos_list)
        posk = pos_list(k); %current windows anchor
        %1 gram
        for j = posk:min([posk+win_len-1 length(seq)])
            jind = j-posk+1;
            c1(jind,seq(j)) = c1(jind,seq(j)) + 1;
        end
        %2 gram
        for j = posk:min([posk+win_len-1 length(seq)])-1
            jind = j-posk+1;
            c2(jind,seq(j), seq(j+1)) = c2(jind,seq(j), seq(j+1)) + 1;
        end
    end
end
for j = 1:win_len
    p1(j,:) = c1(j,:)/sum(c1(j,:));
end
for j = 1:win_len-1
    p2(j,:) = c2(j,:)/sum(c2(j,:));
end
function [num_bps_vals,num_bps_ps] = num_bps_model_hist_list(mfes,anti_inds,model,wps)
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(anti_inds))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
beta = 0.5;
win_len = model.win_len;
num_bps = [];
for i=1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    ai = anti_inds{i};
    is_paired = (ai~=0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
    end
end

```

```

    numpaired5 = sum(is_paired(pos5_on_arm5:pos3_on_arm5));
    numpaired3 = sum(is_paired(pos5_on_arm3:pos3_on_arm3));
    num_bps = [num_bps,min(numpaired5,numpaired3)];
end
end
num_bps_vals = 0:model.win_num_bins_num_bps-1;
n = hist(num_bps,num_bps_vals);
n = n+beta;
num_bps_ps = n/sum(n);
%figure;bar(num_bps_vals,num_bps_ps);title('numbps hist training');
% general params
model_params.win_len = 22; % in nts.
% win params
model_params.win_base_pair_states = 6; % this param is used only for win prediction.
model_params.min_win_bp = 14; % do not allow window to start in bp lower than this.
model_params.win_bulge = 0; % for win prediction. which bulges to look at. 1/2 - bulges1/2, else total
model_params.win_nuc_order = 2; % for positional nuc in win
model_params.win_nuc_pos_win = 15; % for nuc_positional how far in window to look. put win_len for all window.
model_params.win_num_bins_sym = model_params.win_len;
model_params.win_num_bins_num_bps = model_params.win_len;
model_params.win_use_loopdist = 1;
model_params.win_use_win_sym = 1;
model_params.win_use_pos_bulge = 1;
model_params.win_use_num_bps = 1;
model_params.win_use_base_pair = 1;
model_params.win_use_nuc = 1;
% for prediction of pos_given_win
% if the below 2 params are both 0 only looks at the pos5.
model_params.possible_pos_away = 0; % how many to go from 5pos in direction away from loop
    % when searching for positions.
    % note that 0 doesn't go back at all.model_params.
model_params.possible_pos_to = 0; % same but towards loop
model_params.pos_nuc_order = 2; % nuc order for positional nuc
model_params.win_len_for_pos_nuc = 3; % size of win to count nucs. if win_len then looks at whole window
model_params.pos_bulge = 0; % which bulges to look at 1,2 or 0 for the total.
model_params.pos_base_pair_states = 6;
model_params.pos_use_loopdist = 1;
model_params.pos_use_pos_nuc = 1;
model_params.pos_use_pos_bulge = 0;
model_params.pos_use_base_pair = 1;

% general params
model_params.win_len = 22; % in nts.
% win params
model_params.win_base_pair_states = 6; % this param is used only for win prediction.
model_params.min_win_bp = 14; % do not allow window to start in bp lower than this.
model_params.win_bulge = 0; % for win prediction. which bulges to look at. 1/2 - bulges1/2, else total
model_params.win_nuc_order = 2; % for positional nuc in win
model_params.win_nuc_pos_win = 15; % for nuc_positional how far in window to look. put win_len for all window.
model_params.win_num_bins_sym = model_params.win_len;

```

```

model_params.win_num_bins_num_bps = model_params.win_len;
model_params.win_use_loopdist = 1;
model_params.win_use_win_sym = 1;
model_params.win_use_pos_bulge = 1;
model_params.win_use_num_bps = 1;
model_params.win_use_base_pair = 1;
model_params.win_use_nuc = 1;
% for prediction of pos_given_win
% if the below 2 params are both 0 only looks at the pos5.
model_params.possible_pos_away = 0; % how many to go from 5pos in direction away from loop
    % when searching for positions.
    % note that 0 doesn't go back at all.model_params.
model_params.possible_pos_to = 0; % same but towards loop
model_params.pos_nuc_order = 2; % nuc order for positional nuc
model_params.win_len_for_pos_nuc = 3; % size of win to count nucs. if win_len then looks at whole window
model_params.pos_bulge = 0; % which bulges to look at 1,2 or 0 for the total.
model_params.pos_base_pair_states = 6;
model_params.pos_use_loopdist = 1;
model_params.pos_use_pos_nuc = 1;
model_params.pos_use_pos_bulge = 0;
model_params.pos_use_base_pair = 1;

```

```

function p_bp = pos_base_pair_model_list(model,seqs,anti_inds,positions)

```

```

%function p_bp = base_pair_model_list(model,seqs,anti_inds,positions)

```

```

%learns a nonpositional model of base pairs

```

```

% positions{i} is the list of positions on seqs{i}

```

```

% will work also if positions is a vector and not a cell

```

```

win_len = model.win_len;

```

```

numseqs = length(positions);

```

```

if(numseqs~=length(seqs) | numseqs~=length(anti_inds))

```

```

    error('number of seqs or anti_inds differs from length(positions)');

```

```

end

```

```

% transform positions into cell if it is not so.

```

```

if(~iscell(positions))

```

```

    for i=1:numseqs

```

```

        tt{i} = positions(i);

```

```

    end

```

```

    positions = tt;

```

```

end

```

```

seqsbp = nuc2bp(seqs,anti_inds,model.pos_base_pair_states);

```

```

c_bp = zeros(1,model.pos_base_pair_states);

```

```

for i = 1:numseqs

```

```

    seqbp = seqsbp{i};

```

```

    pos_list = positions{i};

```

```

    for k = 1:length(pos_list)

```

```

        posk = pos_list(k); %current windows anchor

```

```

        inds = posk:min([posk+win_len-1 length(seqbp)]);

```

```

        for j = 1:model.pos_base_pair_states

```

```

            c_bp(j) = c_bp(j)+sum(seqbp(inds) == j);

```

```

        end

```

```

    end
end
p_bp = c_bp/sum(c_bp);
function [pb1,pb2,pbtot] = pos_bulge_pos_model_list(model,bulges1,bulges2,positions);
% function [pb1,pb2,pbtot] = pos_bulge_pos_model_list(model,bulges1,bulges2,positions);
% learns a bulge positional model of a list of positions
% positions{i} is the list of positions on seqs{i}
% will work also if positions is a vector and not a cell
win_len = model.win_len;
numseqs = length(positions);
if(numseqs~=length(bulges1) | numseqs~=length(bulges2))
    error('number of bulges differs from length(positions)');
end
% transform positions into cell if it is not so.
if(~iscell(positions))
    for i=1:numseqs
        tt{i} = positions(i);
    end
    positions = tt;
end
for i = 1:numseqs
    b1 = bulges1{i};
    b2 = bulges2{i};
    btot{i} = b1+b2;
end
pb1 = bulge_positional(model,bulges1,positions);
pb2 = bulge_positional(model,bulges2,positions);
pbtot = bulge_positional(model,btot,positions);
function p = bulge_positional(model,bulges,positions)
win_len = model.win_len;
c = zeros(win_len,2);
p = zeros(win_len,1);
for i = 1:length(bulges)
    bulgesi = bulges{i};
    pos_list = positions{i};
    for k = 1:length(pos_list)
        posk = pos_list(k); %current windows anchor
        inds = posk:min([posk+win_len-1 length(bulgesi)]);
        for j=1:length(inds)
            this_ind = inds(j);
            c(j,1) = c(j,1) + bulgesi(this_ind);
            c(j,2) = c(j,2) + (1-bulgesi(this_ind));
        end
    end
end
end
for j = 1:win_len
    p(j) = c(j,1)/sum(c(j,:));
end
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot,minbp)

```



```

% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot,minbp)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
% minbp is the minimal number of basepair required for a legal pal.
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
while ~feof(fid) & seq_no < seqtot
    this_pal_id = str2double(fgetl(fid));
    this_energy = str2double(fgetl(fid));
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    if isempty(line)
        line = 'emptyline';
        fault_seq_emptyline = 1;
    else
        fault_seq_emptyline = 0;
    end
    while(line(1)~= '|') % if emptyline this is always true so will go into loop
        i = i+1;
        structure(i,1:length(line)) = line;
        line = fgetl(fid);
        if isempty(line)
            line = 'emptyline';
            fault_seq_emptyline = 1;
        end
    end
end
if(i~=4)
    fault_seq_numlines = 1;
else
    fault_seq_numlines = 0;
end

fault_seq_struct = 1; % guilty until proven innocent
fault_seq_nuc = 1;
fault_seq_minbp = 1;
if(fault_seq_numlines == 0 & fault_seq_emptyline==0)
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
    if(fault_seq_struct==0)
        % this is the old bulge1 and bulge2, now need to correct that
    end
end

```

```

    bulge_nonsymi=bulge1i;
    bulge_symi=bulge2i;
    for j = 1:length(seqi)
        if(bulge_nonsymi(j))
            if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                bulge_symi(j) = 1;
                bulge_nonsymi(j) = 0;
            end
        end
    end
    for j = length(seqi):-1:1
        if(bulge_nonsymi(j))
            if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                bulge_symi(j) = 1;
                bulge_nonsymi(j) = 0;
            end
        end
    end
    [intseq, fault_seq_nuc] = nuc2int4_new(seqi);
    this_mfe = anti_inds_to_mfe(anti_indi);
    n_bps = size(this_mfe,1);
    if(n_bps < minbp)
        fault_seq_minbp = 1;
    else
        fault_seq_minbp = 0;
    end
end
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & ...
    fault_seq_emptyline == 0 & fault_seq_minbp == 0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    if(fault_seq_emptyline)
        disp(['reason is that there was an empty line in zucker']);
    elseif(fault_seq_numlines)
        disp(['reason is that there were not 4 lines in the draw']);
    elseif(fault_seq_struct)
        disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
    elseif(fault_seq_nuc)

```

```

        disp(['reason is that there was an illegal letter in the seq']);
elseif(fault_seq_minbp)
    disp(['reason is that there were less basepairs then minbp']);
end
counter = counter + 1;
all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1);
        fault_seq = 1;
        seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
        return;
    end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));

```

```

lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col = max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function run_2stage_2pred()
%infile = 'c:\rosetta\data_baseline_29_7\zucker_draw_h152_pipe.txt';
infile = 'C:\rosetta\criteria_for_paper\tests\Zucker_Draw_7pals.txt';
outfile = 'C:\rosetta\criteria_for_paper\tests\out_7pals.txt';
model_filename = 'model_hmdc440_sanger_09_09_03_params1.mat';
fit_filename_both = 'fitfile_mfold3_use_bothsides_hmdc440_sanger_09_09_03_params1.mat';
fit_filename_best = 'fitfile_mfold3_use_bestsides_hmdc440_sanger_09_09_03_params1.mat';
fidin = fopen(infile,'r');
fidout = fopen(outfile,'w');

```

```

seqstot = 1000; %number of sequences to classify each loop
load(model_filename);
while ~feof(fidin)
    disp('reading structure...');
    [palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
        read_struct_minbp(fidin,seqstot,model.min_win_bp);
    mfes = anti_inds_to_mfe(anti_inds);
    [win_pos_est,win_score] = bayes_predict_win(model,palseq,anti_inds,bulges1,bulges2,endbulges);
    score = win_score;
    % use estimated win_pos for prediction of pos!
    [pos_est,pos_score]
    =bayes_predict_pos_given_win(palseq,win_pos_est,anti_inds,bulges1,bulges2,endbulges,model);

    clear pos_est_arm5 pos_est_arm3 pos_est_first pos_est_second res
    for i=1:length(win_score)
        mfe = mfes{i};
        pos_est_arm5(i) = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));
        pos_est_arm3(i) = mfe(win_pos_est(i),2);
        if(pos_est(i)==pos_est_arm5(i))
            pos_est_first(i) = pos_est_arm5(i);
            pos_est_second(i) = pos_est_arm3(i);
        elseif(pos_est(i)==pos_est_arm3(i))
            pos_est_first(i) = pos_est_arm3(i);
            pos_est_second(i) = pos_est_arm5(i);
        else
            disp('something is wrong: pos_est must be either pos_est_arm5 or pos_est_arm3. giving nan!');
            pos_est_first(i) = nan;
            pos_est_second(i) = nan;
        end
    end
end

% infer probabilities
[yside, yprec2_both] = interpolate_prob_new(score, fit_filename_both);
[yside, yprec2_best] = interpolate_prob_new(score, fit_filename_best);

%write to file
%seq_id0 is added so as to sequential order of sequence numbers
res = [pal_id; pos_est_first; pos_est_second; score; yprec2_both;yprec2_best];
fprintf(fidout, '%d %d %d %g %g %g\r\n', res);
end
fclose(fidin);
fclose(fidout);
function [pal_id,pos_est_first,pos_est_second,score,yprec2_both,yprec2_best] =
run_2stage_2pred_giveout(palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy)
model_filename = 'model_hmdc440_sanger_09_09_03_params1.mat';
fit_filename_both = 'fitfile_mfold3_use_bothsides_hmdc440_sanger_09_09_03_params1.mat';
fit_filename_best = 'fitfile_mfold3_use_bestside_hmdc440_sanger_09_09_03_params1.mat';
load(model_filename);
mfes = anti_inds_to_mfe(anti_inds);
[win_pos_est,win_score] = bayes_predict_win(model,palseq,anti_inds,bulges1,bulges2,endbulges);

```

```

score = win_score;
% use estimated win_pos for prediction of pos!
[pos_est,pos_score]
= bayes_predict_pos_given_win(palseq,win_pos_est,anti_inds,bulges1,bulges2,endbulges,model);
for i=1:length(win_score)
    mfe = mfes{i};
    pos_est_arm5(i) = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));
    pos_est_arm3(i) = mfe(win_pos_est(i),2);
    if(pos_est(i)==pos_est_arm5(i))
        pos_est_first(i) = pos_est_arm5(i);
        pos_est_second(i) = pos_est_arm3(i);
    elseif(pos_est(i)==pos_est_arm3(i))
        pos_est_first(i) = pos_est_arm3(i);
        pos_est_second(i) = pos_est_arm5(i);
    else
        disp('something is wrong: pos_est must be either pos_est_arm5 or pos_est_arm3. giving nan!');
        pos_est_first(i) = nan;
        pos_est_second(i) = nan;
    end
end
% infer probabilities
[yside, yprec2_both] = interpolate_prob_new(score, fit_filename_both);
[yside, yprec2_best] = interpolate_prob_new(score, fit_filename_best);
data_dir = 'data_baseline_29_7';
%set_name = 'h152';
%fid = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '_pipe.txt'],'r');
set_name = 'hmdc440_sanger_09_09_03';
fid = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '.txt'],'r');
[palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
    read_structure_with_id_fid(fid,1000);
fclose(fid);
if(length(pal_id)~=length(all_pal_ids))
    error('in human data do not allow faulty seqs, take out of there');
end
mfes = anti_inds_to_mfe(anti_inds);
fname = ['c:\rosetta\data_baseline_29_7\mirseq_' set_name '.txt'];
[mirseq,mirlen] = read_seq_with_id(fname);
mirpos = locate_dicer(mirseq,palseq);
extension = [set_name '_mfold3_params1'];
param_file='params1';
params1;
model = model_params;
model = bayes_learn_win(palseq,anti_inds,bulges1,bulges2,endbulges,mirpos,mirlen,model);
model = bayes_learn_pos_given_win(palseq,anti_inds,bulges1,bulges2,endbulges,mirpos,mirlen,model);
eval(['save model_' extension '.mat model']);
mfold = 3;
mfold_cv_random;
% chooses the correct side to only test win prediction and not side prediction
for i=1:length(mirpos)
    mfe = mfes{i};

```

```

pos_est_arm5(i) = max(1,(mfe(win_pos_est(i),1) - model.win_len + 1));
pos_est_arm3(i) = mfe(win_pos_est(i),2);
d5 = abs(pos_est_arm5(i)-mirpos(i));
d3 = abs(pos_est_arm3(i)-mirpos(i));
pos_error(i) = min(d5,d3);
if(d3<d5)
    pos_est_side_known(i) = pos_est_arm3(i);
else
    pos_est_side_known(i) = pos_est_arm5(i);
end
end
score=win_score;
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est,score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
eval(['print -djpeg use_bestsides_' extension '.jpeg']);
eval(['save fitfile_use_bestsides_' extension '.mat xs ys xp2 yp2']);
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est_side_known,score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est_side_known,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
eval(['print -djpeg use_bothsides_' extension '.jpeg']);
eval(['save fitfile_use_bothsides_' extension '.mat xs ys xp2 yp2']);
figure;
fid = fopen(['info_and_criteria_' extension '.txt'],'w');
thresh_vec = [0:0.01:1];
clf:[thresh,acc2_bestsides,captures] = analyse_errors_thresh_B(pos_est,score,mirpos,endbulges,thresh_vec);
clf:[thresh,acc2_bothsides,captures] =
analyse_errors_thresh_B(pos_est_side_known,score,mirpos,endbulges,thresh_vec);
grid
legend('off')
fprintf(fid,'%%%thresh\tacc2_bothsides\tacc2_bestsides\tcaptures\r\n');
for i=1:length(thresh)

```

```

fprintf(fid,'%1.4f\t%1.4f\t%1.4f\t%d\r\n',thresh(i),acc2_bothsides(i),acc2_bestside(i),captures(i));
end
fclose(fid);
data_dir = 'data_baseline_29_7';
set_name = 'h152';
fid = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '_pipe.txt'],'r');
%set_name = 'hmdc440_sanger_09_09_03';
%fid = fopen(['c:\rosetta\data_baseline_29_7\zucker_draw_' set_name '.txt'],'r');
[palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
    read_structure_with_id_fid(fid,1000);
fclose(fid);
if(length(pal_id)~=length(all_pal_ids))
    error('in human data do not allow faulty seqs, take out of there');
end
mfes = anti_inds_to_mfe(anti_inds);
fname = ['c:\rosetta\data_baseline_29_7\mirseq_' set_name '.txt'];
[mirseq,mirlen] = read_seq_with_id(fname);
mirpos = locate_dicer(mirseq,palseq);
extension = [set_name '_proto4_params1'];
params1;
model = model_params;
model = bayes_learn_win(palseq,anti_inds,bulges1,bulges2,endbulges,mirpos,mirlen,model);
model = bayes_learn_pos_given_win(palseq,anti_inds,bulges1,bulges2,endbulges,mirpos,mirlen,model);
eval(['save model_' extension '.mat model']);
mfold = 3;
maxd=4;
mfold_cv_proto;
mfes_e = mfes(examples);
mirpos_e = mirpos(examples);
win_score_e = win_score(examples);
pos_est_e = pos_est(examples);
win_pos_est_e = win_pos_est(examples);
endbulges_e = endbulges(examples);
% chooses the correct side to only test win prediction and not side prediction
for i=1:length(examples)
    mfe = mfes_e{i};
    pos_est_arm5(i) = max(1,(mfe(win_pos_est_e(i),1) - model.win_len + 1));
    pos_est_arm3(i) = mfe(win_pos_est_e(i),2);
    d5 = abs(pos_est_arm5(i)-mirpos_e(i));
    d3 = abs(pos_est_arm3(i)-mirpos_e(i));
    pos_error(i) = min(d5,d3);
    if(d3<d5)
        pos_est_side_known_e(i) = pos_est_arm3(i);
    else
        pos_est_side_known_e(i) = pos_est_arm5(i);
    end
end
score_e=win_score_e;
figure
subplot(2,1,1)

```



```

res = analyse_errors_perc(pos_est_e,score_e,mirpos_e,endbulges_e);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est_e,score_e,mirpos_e,endbulges_e,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
eval(['print -djpeg use_bestsides_' extension '.jpeg']);
eval(['save fitfile_use_bestsides_' extension '.mat xs ys xp2 yp2']);
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est_side_known_e,score_e,mirpos_e,endbulges_e);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est_side_known_e,score_e,mirpos_e,endbulges_e,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
eval(['print -djpeg use_bothsides_' extension '.jpeg']);
eval(['save fitfile_use_bothsides_' extension '.mat xs ys xp2 yp2']);
figure;
fid = fopen(['info_and_criteria_' extension '.txt'],'w');
thresh_vec = [0:0.01:1];
clf;[thresh,acc2_bestsides,captures] =
analyse_errors_thresh_B(pos_est_e,score_e,mirpos_e,endbulges_e,thresh_vec);
clf;[thresh,acc2_bothsides,captures] =
analyse_errors_thresh_B(pos_est_side_known_e,score_e,mirpos_e,endbulges_e,thresh_vec);
grid
legend('off')
fprintf(fid,'%%%thresh\tacc2_bothsides\tacc2_bestsides\tcaptures\r\n');
for i=1:length(thresh)
    fprintf(fid,'%1.4f\t%1.4f\t%1.4f\t%1.4f\t\r\n',thresh(i),acc2_bothsides(i),acc2_bestsides(i),captures(i));
end
fclose(fid);
function [p_bp_arm5,p_bp_arm3] = win_base_pair_model_list(mfes,anti_inds,seqs,model,wps)
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(anti_inds) | numseqs~=length(seqs))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
end

```

```

    wps = tt;
end
win_len = model.win_len;
base_pair_states = model.win_base_pair_states;
c_bp_arm5 = zeros(1,base_pair_states);
c_bp_arm3 = zeros(1,base_pair_states);
seqsbp = nuc2bp(seqs,anti_inds,base_pair_states);
for i = 1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    ai = anti_inds{i};
    is_paired = (ai~=0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
        for j = 1:base_pair_states
            c_bp_arm5(j) = c_bp_arm5(j)+sum(seqsbp{i}(pos5_on_arm5:pos3_on_arm5) == j);
            c_bp_arm3(j) = c_bp_arm3(j)+sum(seqsbp{i}(pos5_on_arm3:pos3_on_arm3) == j);
        end
    end
end
p_bp_arm5 = c_bp_arm5/sum(c_bp_arm5);
p_bp_arm3 = c_bp_arm3/sum(c_bp_arm3);
function [pb_arm5,pb_arm3,pb1_arm5,pb1_arm3,pb2_arm5,pb2_arm3] = ...
    win_bulge_pos_model_list(mfes,bulges1,bulges2,model,wps)
% on both sides of window from loop end of window
% pb1 - for bulges1 pb2 - for bulges2 pb - for total
win_len = model.win_len;
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(bulges1) | numseqs~=length(bulges2))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
for i=1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    bulges{i} = bulges1{i}+bulges2{i};
    inds5_i = cell(0);
    inds3_i = cell(0);
    for k=1:length(wp_list)
        wp = wp_list(k);

```

```

pos3_on_arm5 = mfe(wp,1);
pos5_on_arm3 = mfe(wp,2);
pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
pos3_on_arm3 = min(length(bulges{i}),pos5_on_arm3+win_len-1);
inds5_i{k} = pos3_on_arm5:-1:pos5_on_arm5; % always start from loop side
inds3_i{k} = pos5_on_arm3:pos3_on_arm3;
end
inds5{i} = inds5_i;
inds3{i} = inds3_i;
end
pb_arm5 = bulge_positional_list(model,bulges,inds5);
pb_arm3 = bulge_positional_list(model,bulges,inds3);
pb1_arm5 = bulge_positional_list(model,bulges1,inds5);
pb1_arm3 = bulge_positional_list(model,bulges1,inds3);
pb2_arm5 = bulge_positional_list(model,bulges2,inds5);
pb2_arm3 = bulge_positional_list(model,bulges2,inds3);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function p = bulge_positional_list(model,bulges,inds)
win_len = model.win_len;
c = zeros(win_len,2);
p = zeros(win_len,1);
for i = 1:length(bulges)
    bulgesi = bulges{i};
    for k = 1:length(inds{i})
        this_inds = inds{i}{k};
        for j=1:length(this_inds)
            this_ind = this_inds(j);
            c(j,1) = c(j,1) + bulgesi(this_ind);
            c(j,2) = c(j,2) + (1-bulgesi(this_ind));
        end
    end
end
end
for j = 1:win_len
    p(j) = c(j,1)/sum(c(j,:));
end
function [p1_5,p2_5,p1_3,p2_3] = win_nuc_positional_model_list(seqs,mfes,model,wps)
win_len = model.win_len;
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(seqs))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
beta = 0.5;

```

```

Ns = 4; %number of states
c1_5 = zeros(win_len,Ns);
c2_5 = beta*ones(win_len-1,Ns,Ns);
c1_3 = zeros(win_len,Ns);
c2_3 = beta*ones(win_len-1,Ns,Ns);
for i = 1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    seqsi = seqs{i};
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(seqsi),pos5_on_arm3+win_len-1);
        inds5 = pos5_on_arm5:pos3_on_arm5;
        inds3 = pos5_on_arm3:pos3_on_arm3;
        seq5 = seqsi(inds5);
        seq3 = seqsi(inds3);

        %1 gram
        for j = 1:length(seq5)
            c1_5(j,seq5(j)) = c1_5(j,seq5(j)) + 1;
        end
        %2 gram
        for j = 1:length(seq5)-1
            c2_5(j,seq5(j),seq5(j+1)) = c2_5(j,seq5(j), seq5(j+1)) + 1;
        end

        %1 gram
        for j = 1:length(seq3)
            c1_3(j,seq3(j)) = c1_3(j,seq3(j)) + 1;
        end
        %2 gram
        for j = 1:length(seq3)-1
            c2_3(j,seq3(j),seq3(j+1)) = c2_3(j,seq3(j), seq3(j+1)) + 1;
        end
    end
end
for j = 1:win_len
    p1_5(j,:) = c1_5(j,:)/sum(c1_5(j,:));
    p1_3(j,:) = c1_3(j,:)/sum(c1_3(j,:));
end
for j = 1:win_len-1
    p2_5(j,:) = c2_5(j,:)/sum(c2_5(j,:));
    p2_3(j,:) = c2_3(j,:)/sum(c2_3(j,:));
end
function [win_sym_vals,win_sym_ps] = win_sym_model_list(mfes,anti_inds,model,wps)
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(anti_inds))

```

```

    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
beta = 0.5;
win_len = model.win_len;
win_sym = [];
for i=1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    ai = anti_inds{i};
    is_paired = (ai~=0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
        numunpaired5 = sum(~is_paired(pos5_on_arm5:pos3_on_arm5));
        numunpaired3 = sum(~is_paired(pos5_on_arm3:pos3_on_arm3));
        win_sym = [win_sym,abs(numunpaired5-numunpaired3)];
    end
end
win_sym_vals = 0:model.win_num_bins_sym-1;
n = hist(win_sym,win_sym_vals);
n = n+beta;
win_sym_ps = n/sum(n);
%figure;bar(win_sym_vals,win_sym_ps);title('win sym training');

```

```

function res = analyse_errors_perc(pos_estimated,score,pos, endbulges)
%analyse_errors_perc(pos_estimated,score,pos, endbulges)
% measure the distribution of erros
N = 100;
perc = [1:-1/N:0]*100;
thresh = prctile(score, perc);
accuracy = zeros(0);
correct_side_dist1 = zeros(0); %correct size, distance = 1;
correct_side_dist2 = zeros(0);
correct_side_dsth = zeros(0);
wrong_side = zeros(0);
fraction = zeros(0);
count = 0;
N = length(pos);
for i = 1:length(endbulges)
    eb = find(endbulges{i});
    correct_side(i) = 0.5*( 1 + sign((pos_estimated(i) - eb(1))*(pos(i) -eb(1)))); %one for correct side estimate
end
for i = 1:length(thresh)
    I = find(score >= thresh(i));
    if ~isempty(I)
        count = count + 1;
        accuracy(count) = sum(pos_estimated(I) == pos(I))/length(I);

        J1 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 1);
        correct_side_dist1(count) = length(J1)/length(I);
        J2 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 2);
        correct_side_dist2(count) = length(J2)/length(I);
        J3 = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) == 3);
        correct_side_dist3(count) = length(J3)/length(I);
        Jh = find(correct_side(I) & abs(pos(I)- pos_estimated(I)) > 3);
        correct_side_dsth(count) = length(Jh)/length(I);

        wrong_side(count) = sum(1-correct_side(I))/length(I);

        fraction(count) = length(I)/N;
    else
        count = count+1;
        accuracy(count) = NaN;
        correct_side_dist1(count) = NaN;
        correct_side_dist2(count) = NaN;
        correct_side_dsth(count) = NaN;
        wrong_side(count) = NaN;
        fraction(count) = NaN;
    end
end

acc1 = accuracy + correct_side_dist1;
acc2 = accuracy + correct_side_dist1 + correct_side_dist2;
acc3 = accuracy + correct_side_dist1 + correct_side_dist2 + correct_side_dist3;

```

```

%clf
hold on

plot(perc, acc3,'y','linewidth',2)
plot(perc, acc2,'g','linewidth',2)
plot(perc, acc1,'r','linewidth',2)
plot(perc, accuracy,'b','linewidth',2)
plot(perc, wrong_side,'k','linewidth',2)
plot(perc, thresh,'c','linewidth',2)
legend('dist \leq 3','dist \leq 2', 'dist \leq 1', 'precise', 'wrong side', 'threshold',2);
xlabel('percentage');
axis([0 100 0 1]);

%keyboard
%prepare result
N = length(accuracy);
res = [accuracy(N), acc1(N), acc2(N), acc3(N), 1-wrong_side(N), acc2(round(0.2*N))];
return
function mfe = anti_inds_to_mfe(anti_inds)
% anti_inds holds for each nuc in the seq what is the index of
% the nuc across from it where the 0 means unpaired (this is returned by read_structure_withanti).
% returns mfe which is the structure in the format of rnafold, i.e. only base pairs:
% mfe is a 2 col matrix, the first being the bases on arm5 which are paired and the second
% their corresponding pairs
if(~iscell(anti_inds))
    mfe = get_mfe(anti_inds);
    return;
end
for i=1:length(anti_inds)
    mfe{i} = get_mfe(anti_inds{i});
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function mfe = get_mfe(ai)
bps=0;
for i=1:length(ai)
    if(ai(i))
        if(i>ai(i))
            return
        end
        bps = bps+1;
        mfe(bps,1) = i;
        mfe(bps,2) = ai(i);
    end
end
end
%ktup, k, alpha
param_sets = [8,4,0.2;
    8,4,0.25;
    8,4,0.3;
    8,5,0.2;

```

```

8,5,0.25;
8,5,0.3;
9,4,0.2;
9,4,0.25;
9,4,0.3];
fid = fopen('batch_results_proto4_A.txt','w');
params1;
maxd = 4;
set_name = model_params.trained_on;
fid = fopen(['zucker_draw_' set_name '.txt'],'r');
[palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
    read_structure_with_id_fid(fid,1000);
fclose(fid);
if(length(pal_id)~=length(all_pal_ids))
    error('in training data do not allow faulty seqs, take out of there');
end
mfes = anti_inds_to_mfe(anti_inds);
fname = ['mirseq_' set_name '.txt'];
[mirseq,mirlen] = read_seq_with_id(fname);
mirpos = locate_dicer(mirseq,palseq);
filename = ['clust_proto_members_' num2str(maxd) '_' set_name '.txt'];
clust_num = load(filename);
if length(clust_num) ~= length(palseq)
    error('clust_num wrong size');
end
for i=1:size(params_sets,1)
    model_params.ktup = param_sets(i,1);
    model_params.k = param_sets(i,2);
    model_params.alpha = param_sets(i,3);
    [pos_est,edist_score,win_score] = mfold_cv_proto_members(mirseq,mirpos,mirlen,palseq,anti_inds,...
        bulges1,bulges2,endbulges,clust_num,model_params);
    score = edist_score; %!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
    res = analyse_errors_perc(pos_est,score,mirpos,endbulges);
    fprintf(fid,'%d %d %4.2f %5.3f %5.3f %5.3f %5.3f %5.3f\r\n', model_params.ktup, model_params.k, ...
        model_params.alpha,res(1),res(2),res(3),res(5),res(6));
end
fclose(fid);
function model = bayes_learn_win(seqs,anti_inds,bulges1,bulges2,endbulges,pos,mirlen,model)
%model_params is a struct.
ds_win_len = model.ds_win_len;
% mfes{i} holds the structure in the basepair notation
mfes = anti_inds_to_mfe(anti_inds);
% win_pos(i) is the position of the window corresponding to mir i
if(model.use_mirlen_in_learning_win)
    win_pos = get_win_pos_v1(mfes,anti_inds,pos,mirlen);
else
    win_pos = get_win_pos_v1(mfes,anti_inds,pos,ds_win_len*ones(size(pos)));
end
% for each seq hold the mirposition and all possible positions that are not mirpos
for i=1:length(pos)

```



```

mirwin(i) = win_pos(i);
ai = anti_inds{i};
mfe = mfes{i};
n_bps = size(mfes{i},1);
tt = setdiff([1:n_bps],mirwin(i));
nonmirwins_legal = [];
for j=1:length(tt)
    wp=tt(j);
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    if((pos3_on_arm5>=model.min_win_len) & (length(ai)-pos5_on_arm3+1>=model.min_win_len))
        nonmirwins_legal = [nonmirwins_legal,wp];
    end
end
nonmirwin{i} = nonmirwins_legal;
end
[mean_loopdist,std_loopdist] = loopdist_bp_model_normal(win_pos,mfes);
model.mean_loopdist_bp = mean_loopdist;
model.std_loopdist_bp = std_loopdist;
[win_num_bps_mir_vals,win_num_bps_mir_ps] = num_bps_model_hist_list(mfes,anti_inds,model,mirwin);
[win_num_bps_nonmir_vals,win_num_bps_nonmir_ps] = num_bps_model_hist_list(mfes,anti_inds,model,nonmirwin);
model.win_num_bps_mir_vals = win_num_bps_mir_vals;
model.win_num_bps_mir_ps = win_num_bps_mir_ps;
model.win_num_bps_nonmir_vals = win_num_bps_nonmir_vals;
model.win_num_bps_nonmir_ps = win_num_bps_nonmir_ps;
[win_sym_mir_vals,win_sym_mir_ps] = win_sym_model_list(mfes,anti_inds,model,mirwin);
[win_sym_nonmir_vals,win_sym_nonmir_ps] = win_sym_model_list(mfes,anti_inds,model,nonmirwin);
model.win_sym_mir_vals = win_sym_mir_vals;
model.win_sym_mir_ps = win_sym_mir_ps;
model.win_sym_nonmir_vals = win_sym_nonmir_vals;
model.win_sym_nonmir_ps = win_sym_nonmir_ps;
[pb_arm5_mir,pb_arm3_mir,pb1_arm5_mir,pb1_arm3_mir,pb2_arm5_mir,pb2_arm3_mir]...
    = win_bulge_pos_model_list(mfes,bulges1,bulges2,model,mirwin);
[pb_arm5_nonmir,pb_arm3_nonmir,pb1_arm5_nonmir,pb1_arm3_nonmir,pb2_arm5_nonmir,pb2_arm3_nonmir]...
    = win_bulge_pos_model_list(mfes,bulges1,bulges2,model,nonmirwin);
model.win_bulge_posit_arm5_mir = pb_arm5_mir;
model.win_bulge_posit_arm3_mir = pb_arm3_mir;
model.win_bulge1_posit_arm5_mir = pb1_arm5_mir;
model.win_bulge1_posit_arm3_mir = pb1_arm3_mir;
model.win_bulge2_posit_arm5_mir = pb2_arm5_mir;
model.win_bulge2_posit_arm3_mir = pb2_arm3_mir;
model.win_bulge_posit_arm5_nonmir = pb_arm5_nonmir;
model.win_bulge_posit_arm3_nonmir = pb_arm3_nonmir;
model.win_bulge1_posit_arm5_nonmir = pb1_arm5_nonmir;
model.win_bulge1_posit_arm3_nonmir = pb1_arm3_nonmir;
model.win_bulge2_posit_arm5_nonmir = pb2_arm5_nonmir;
model.win_bulge2_posit_arm3_nonmir = pb2_arm3_nonmir;
[win_p_bp_arm5_mir,win_p_bp_arm3_mir] = ...
    win_base_pair_model_list(mfes,anti_inds,seqs,model,mirwin);
[win_p_bp_arm5_nonmir,win_p_bp_arm3_nonmir] = ...

```

```

win_base_pair_model_list(mfes,anti_inds,seqs,model,nonmirwin);
model.win_base_pair_arm5_mir = win_p_bp_arm5_mir;
model.win_base_pair_arm3_mir = win_p_bp_arm3_mir;
model.win_base_pair_arm5_nonmir = win_p_bp_arm5_nonmir;
model.win_base_pair_arm3_nonmir = win_p_bp_arm3_nonmir;
return
function [pos,combined_score, edist_score,win_score] = firstkpp_predict_combined(model,
seqs,anti_inds,bulges1,bulges2,endbulges);
% [pos,combined_score,edist_score,win_score] = firstkpp_predict_combined(model,
seqs,anti_inds,bulges1,bulges2,endbulges);
%
% predict best matching miRNA position by edit distance to the first k letters of known mirs
% from the best scoring positions, take the ones with best 2stage score
%
%model contains all learned model, that of bayesian predictor and all known mirs
%seqs is in int format. converted to nucleotide format inside firstkpp_predict1
%
% GD 21.10.03
disp('calculating...');
for i = 1:length(seqs)
    [posi, combined_scorei,edist_scorei, win_scorei] =
firstkpp_predict1(model,seqs{i},anti_inds{i},bulges1{i},bulges2{i},endbulges{i});
    pos(i) = posi;
    combined_score(i) = combined_scorei;
    edist_score(i) = edist_scorei;
    win_score(i) = win_scorei;
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [pos,combined_score, edist_score, win_score] = firstkpp_predict1(model,seqsi,
anti_indsi,bulges1i,bulges2i,endbulgesi);
%calculate the best matching position of dicer
min_win_len = model.min_win_len;
modelk = model.k;
ktup = model.ktup;
gamma = model.gamma;
lb = find(endbulgesi);
eb_begin = lb(1);
eb_end = lb(end);
%initialize variables with the largest possible distance
mean_k = ktup(ones(length(seqsi),1));
seqsi_nuc = int2nuc(seqsi);
%upper side
for i = 1:1:eb_begin-min_win_len
    p = seqsi_nuc(i:i+ktup-1);
    for j = 1:length(model.seqsd)
        d(j) = editD(p,model.seqsd{j});
    end
    % take also the mean of highest percentile

```

```

[ds,l] = sort(d);
mean_k(i) = mean(ds(1:modelk));
end
%lower side
for i = eb_end+1:1:length(seqsi)-min_win_len+1
    p = seqsi_nuc(i:i+ktup-1);
    for j = 1:length(model.seqsd)
        d(j) = editD(p,model.seqsd{j});
    end
    % take also the mean of highest ten percentile
    [ds,l] = sort(d);
    mean_k(i) = mean(ds(1:modelk));
end
%rewrite the last choosing of parameters
fk_score = 1 - model.beta*mean_k/ktup;
max_score = max(fk_score);
thrsh_score = (1-model.alpha)*max_score;
lc = find(fk_score >= thrsh_score);
if isempty(lc)
    pos = nan;
    combined_score = nan;
    edist_score = nan;
    win_score = nan;
    return
end
% now compute two stage scores
twostg_score = win_score_2stagei(model,seqsi,anti_indsi,bulges1i,bulges2i,endbulgesi);
twostg_score = interpolate_nan(twostg_score,endbulgesi);
combined_score = gamma*fk_score(lc) + (1-gamma)*twostg_score(lc);
[max_combined, imx] = max(combined_score);
pos = lc(imx);
combined_score = max_combined;
edist_score = fk_score(pos);
win_score = twostg_score(pos);
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function score_interp = interpolate_nan(score, endbulgesi);
% fill all NaNs which are surrounded by numeric values by interpolation
lb = find(endbulgesi);
score(lb) = 0;
A = find(isnan(score));
B = find(~isnan(score));
score_interp = zeros(size(score));
score_interp(B) = score(B);
score_interp(A) = interp1(B,score(B),A);
score_interp(find(isnan(score_interp))) = 0;
score_interp = score_interp';
return
function win_mirpos = get_win_pos_v1(mfes,anti_inds,mirpos,mirlen)

```

```

% function win_mirpos = get_win_pos(mfes,anti_inds,mirpos,mirlen)
% returns win_mirpos in index of basepair (from legs not loop).
% i.e. mfe(win_mirpos,1) is the nuc pos on the 5 arm
% for mir on arm3 returns the closest bp from its mirpos towards the legs
% for mir on arm5 returns the closest bp from its END (mirpos+mirlen-1) towards the legs
% also towards the legs
for i=1:length(mirpos)
    pos5 = mirpos(i);
    pos3 = pos5+mirlen(i)-1;
    mfe = mfes{i};
    arm5 = mfe(:,1);
    arm3 = mfe(:,2);
    eb_start = arm5(end)+1;
    eb_end = arm3(end)-1;
    eb_len = eb_end-eb_start+1;
    side5 = (pos5<eb_start);
    ai = anti_inds{i};
    is_paired = (ai~=0);
    if(side5)
        k=0;
        while(~is_paired(pos3-k))
            k=k+1;
        end
        win_mirpos(i) = find(arm5==(pos3-k));
    else
        k=0;
        while(~is_paired(pos5+k))
            k=k+1;
        end
        win_mirpos(i) = find(arm3==(pos5+k));
    end
    if isempty(win_mirpos(i))
        error('get_win_pos: fatal error. aborting.');
    end
end

function strseq = int2nuc(intseq, ncase)
%strseq = int2nuc(intseq, ncase)
%convert a sequence of '1 2 3 4' into 'A C T G' or 'a c t g'
% ncase = uppercase | lowercase
if(isletter(intseq(1)))
    strseq = intseq;
    return;
end
if nargin == 1
    ncase = 'uppercase';
end
if strcmp(ncase,'uppercase')
    nucs = 'ACTG';
elseif strcmp(ncase,'lowercase')
    nucs = 'actg';

```

```

end
strseq = char(size(intseq));
for i = 1:length(intseq)
    strseq(i) = nucs(intseq(i));
end
return
function [yside, yprec2] = interpolate_prob_new(score, fitfile);
%[yside, yprec2] = interpolate_prob_new(score, fitfile);
% load the parameters for interpolation
load(fitfile);
%interpolate
yside = interp1(xs,ys,score,'linear');
yprec2 = interp1(xp2,yp2,score,'linear');
% extrapolate if necessary
if(min(xs)==xs(1)) % x is increasing
    yside(score<xs(1)) = ys(1);
    yprec2(score<xp2(1)) = yp2(1);
    yside(score>xs(end)) = ys(end);
    yprec2(score>xp2(end)) = yp2(end);
else % x is decreasing
    yside(score>xs(1)) = ys(1);
    yprec2(score>xp2(1)) = yp2(1);
    yside(score<xs(end)) = ys(end);
    yprec2(score<xp2(end)) = yp2(end);
end
returnfunction [mean_dist,std_dist] = loopdist_bp_model_normal(win_pos,mfes)
for i=1:length(win_pos)
    n_bps = size(mfes{i},1);
    loopdist(i) = n_bps - win_pos(i);
end
% cut off outliers
lp = prctile(loopdist,[2.5 97.5]);
l = find(loopdist >= lp(1) & loopdist <=lp(2));
mean_dist = mean(loopdist(l));
std_dist = std(loopdist(l));
%figure;hist(loopdist,[0:max(loopdist+1)]);title('loopdist training');function [pos_est,score,edist_score,win_score] =
mfold_cv_members(mirseq,mirpos,mirlen,palseq,anti_inds,bulges1,bulges2,...
    endbulges,clust_num,mfold,model_params);
%[pos_est,score,edist_score,win_score] =
mfold_cv_members(mirseq,mirpos,mirlen,palseq,anti_inds,bulges1,bulges2,...
% endbulges,clust_num,mfold,model_params);
n_all = length(palseq);
pos_est = zeros(0);
score =zeros(0);
model = model_params;
clust_list = unique(clust_num);
num_clusts = length(clust_list)
bins = round(0:num_clusts/mfold:num_clusts)
for m=1:mfold
    disp(['m= ' num2str(m)]);

```

```

bs_clusts = clust_list([bins(m)+1: bins(m+1)]);
bs = []; % test set
for i=1:length(bs_clusts)
    this_clust = bs_clusts(i);
    bs = [bs;find(clust_num==this_clust)];
end
disp(['size test set: ' num2str(size(bs))]);
bt = setdiff(1:n_all, bs);% train set

disp('building model...');
% learn model , and add all known mirs to it
model = bayes_learn_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt), ...
    mirpos(bt),mirlen(bt),model);
clear seqsd_train;
for i = 1:length(bt); seqsd_train{i} = mirseq{bt(i)}(1:model.ktup); end
model.seqsd = transform_format(seqsd_train);

disp('predicting...');
[pos_est_m,score_m,edist_score_m,win_score_m] = firstkpp_predict_combined...
    (model, palseq(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs));
pos_est(bs) = pos_est_m;
score(bs) = score_m;
edist_score(bs) = edist_score_m;
win_score(bs) = win_score_m;
end
returnfunction [pos_est,score,edist_score,win_score] =
mfold_cv_random(mirseq,mirpos,mirlen,palseq,anti_inds,bulges1,bulges2,...
    endbulges,mfold,randstate,model_params,permute);
%[pos_est,score,edist_score,win_score] =
mfold_cv_random(mirseq,mirpos,mirlen,palseq,anti_inds,bulges1,bulges2,...
% endbulges,mfold,randstate,model_params,permute);
if(~exist('permute'))
    permute = 1;
end
n_all = length(palseq);
bins = round(0:n_all/mfold:n_all)
bins_all = 1:n_all;
if permute
    rand('state',randstate);
    l = randperm(n_all);
    mirseq = mirseq(l);
    mirpos = mirpos(l);
    mirlen = mirlen(l);
    palseq = palseq(l);
    anti_inds = anti_inds(l);
    bulges1 = bulges1(l);
    bulges2 = bulges2(l);
    endbulges = endbulges(l);
end
pos_est = zeros(0);

```

```

edist_score=zeros(0);
win_score=zeros(0);
model=model_params;
m=1;
while m <= mfold
    bs=[bins(m)+1:bins(m+1)];% test set
    bt=setdiff(bins_all,bs);% train set

    disp(['m = ' num2str(m)]);

    disp('building model...');
    % learn model , and add all known mirs to it
    model=bayes_learn_win(palseq(bt),anti_inds(bt),bulges1(bt),bulges2(bt),endbulges(bt), ...
        mirpos(bt),mirlen(bt),model);
    clear seqsd_train;
    for i=1:length(bt); seqsd_train{i}=mirseq{bt(i)}(1:model.ktup); end
    model.seqsd=transform_format(seqsd_train);
    disp('predicting...');
    [pos_est_m,score_m,edist_score_m,win_score_m]=firstkpp_predict_combined...
        (model,palseq(bs),anti_inds(bs),bulges1(bs),bulges2(bs),endbulges(bs));
    pos_est(bs)=pos_est_m;
    score(bs)=score_m;
    edist_score(bs)=edist_score_m;
    win_score(bs)=win_score_m;

    m=m+1;
end
if permute
    % undo the permutation
    pos_est(l)=pos_est;
    score(l)=score;
    edist_score(l)=edist_score;
    win_score(l)=win_score;
end
returnfunction [intseq,fault_seq]=nuc2int(strseq);
%[intseq,fault_seq]=nuc2int(strseq)
%convert a sequence of 'A C T G' into a array of 1 2 3 4
if(~isletter(strseq(1)))
    intseq=strseq;
    fault_seq=0;
    return;
end
intseq=zeros(size(strseq));
fault_seq=0;
for i=1:length(strseq)
    switch upper(strseq(i))
        case 'A' , intseq(i)=1;
        case 'C' , intseq(i)=2;
        case 'T' , intseq(i)=3;
        case 'G' , intseq(i)=4;
    end
end

```

```

        otherwise , intseq = []; fault_seq = 1; break;
    end
end
function [num_bps_vals,num_bps_ps] = num_bps_model_hist_list(mfes,anti_inds,model,wps)
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(anti_inds))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
beta = 0.5;
win_len = model.ds_win_len;
num_bps = [];
for i=1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    ai = anti_inds{i};
    is_paired = (ai~=0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
        numpaired5 = sum(is_paired(pos5_on_arm5:pos3_on_arm5));
        numpaired3 = sum(is_paired(pos5_on_arm3:pos3_on_arm3));
        num_bps = [num_bps,min(numpaired5,numpaired3)];
    end
end
num_bps_vals = 0:model.win_num_bins_num_bps-1;
n = hist(num_bps,num_bps_vals);
n = n+beta;
num_bps_ps = n/sum(n);
%figure;bar(num_bps_vals,num_bps_ps);title('numbps hist training');
model_params.trained_on = 'hmdcc440';
% see files with this extension for the training data itself
%specific firstk parameters
model_params.ktup = 8; % window size for edist part
model_params.k = 4; % number of nearest neighbors in KNN
model_params.alpha = 0.25; %fraction best score that defines the region for ranking with 2stage
model_params.beta = 2; %scaling parameter: score = 1-beta*mean_k/ktup;
model_params.gamma = 0.75; % the weight of the first (edist) score in combined score
% win params
model_params.min_win_len = 17; % single starnded min win len in nts.
model_params.ds_win_len = 22; % double starnded win len in nts.

```



```

model_params.use_mirlen_in_learning_win = 0; % if 1 uses mirlen else uses win_len in learning win
model_params.win_base_pair_states = 6; % this param is used only for win prediction.
model_params.win_bulge = 0; % for win prediction. which bulges to look at. 1/2 - bulges1/2, else total
model_params.win_num_bins_sym = model_params.ds_win_len;
model_params.win_num_bins_num_bps = model_params.ds_win_len;
model_params.win_use_loopdist = 1;
model_params.win_use_win_sym = 1;
model_params.win_use_pos_bulge = 1;
model_params.win_use_num_bps = 1;
model_params.win_use_base_pair = 0;
function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% function [seqs,anti_inds,bulges_nonsym,bulges_sym,endbulges,pal_id,energy,all_pal_ids] =
read_structure_with_id_fid(fid,seqtot)
% same as read_structure_withanti_fid but reads file that have before the 4 line zucker draw
% a line giving the pal_id and a line giving the energy.
% all_pal_ids is all ids read from file, whether faulty or not
% new feature: checks that draw is not messed up and if it is gives faulty seq.
Mxplen = 250; % maximal length of palindrom
counter = 0;
seq_no = 0;
seqs = cell(0);
bulges_nonsym= cell(0);
bulges_sym= cell(0);
endbulges = cell(0);
pal_id = zeros(0);
energy = zeros(0);
while ~feof(fid) & seq_no < seqtot
    this_pal_id = str2double(fgetl(fid));
    this_energy = str2double(fgetl(fid));
    structure = char(4,250);
    i = 0;
    line = fgetl(fid);
    if isempty(line)
        line = 'emptyline';
        fault_seq_emptyline = 1;
    else
        fault_seq_emptyline = 0;
    end
    while(line(1)~= '|') % if emptyline this is always true so will go into loop
        i = i+1;
        structure(i,1:length(line)) = line;
        line = fgetl(fid);
        if isempty(line)
            line = 'emptyline';
            fault_seq_emptyline = 1;
        end
    end
end
if(i~=4)
    fault_seq_numlines = 1;

```

```

else
    fault_seq_numlines = 0;
end

fault_seq_struct = 1; % guilty until proven innocent
fault_seq_nuc = 1;
if(fault_seq_numlines == 0 & fault_seq_emptyline==0)
    [seqi, anti_indi, bulge1i, bulge2i, endbulgei,fault_seq_struct] = get_features(structure);
    if(fault_seq_struct==0)
        % this is the old bulge1 and bulge2, now need to correct that
        bulge_nonsymi=bulge1i;
        bulge_symi=bulge2i;
        for j = 1:length(seqi)
            if(bulge_nonsymi(j))
                if(bulge_symi(max(1,j-1))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        for j = length(seqi):-1:1
            if(bulge_nonsymi(j))
                if(bulge_symi(min(j+1,length(seqi)))) % a neighbor has a bulgesym flag on
                    bulge_symi(j) = 1;
                    bulge_nonsymi(j) = 0;
                end
            end
        end
        [intseq, fault_seq_nuc] = nuc2int(seqi);
    end
end

if (fault_seq_struct == 0 & fault_seq_nuc == 0 & fault_seq_numlines == 0 & fault_seq_emptyline == 0)
    seq_no = seq_no + 1;
    seqs{seq_no} = intseq;
    anti_inds{seq_no} = anti_indi;
    bulges_nonsym{seq_no} = bulge_nonsymi;
    bulges_sym{seq_no} = bulge_symi;
    endbulges{seq_no} = endbulgei;
    pal_id(seq_no) = this_pal_id;
    energy(seq_no) = this_energy;
    counter = counter + 1;
    all_pal_ids(counter) = this_pal_id;
else
    disp(['faulty seq on pal id ' num2str(this_pal_id)])
    if(fault_seq_emptyline)
        disp(['reason is that there was an empty line in zucker']);
    elseif(fault_seq_numlines)
        disp(['reason is that there were not 4 lines in the draw']);
    elseif(fault_seq_struct)

```

```

        disp(['reason is that draw was messed has nuc in pair and bulge at the same time']);
elseif(fault_seq_nuc)
    disp(['reason is that there was an illegal letter in the seq']);
end
counter = counter + 1;
all_pal_ids(counter) = this_pal_id;
end
end
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [seq, anti_ind, bulge1, bulge2, endbulge, fault_seq] = get_features(structure)
% get sequence as well as bulge structure
fault_seq = 0;
%upper half (5' side)
bulge_row = 1; % the row of bulge letters
bulge_row_opposite = 4;
uphalf = structure(1:2,:);
[j,k] = find(isletter(uphalf));
max_col = max(k);
tmpmat = zeros(2,max_col);
count = 0;
for col =1: max_col
    fl = find(isletter(uphalf(:,col)));
    if (length(fl)>1);
        fault_seq = 1;
        seq=nan;anti_ind=nan;bulge1=nan;bulge2=nan;endbulge=nan;
        return;
    end;
    if ~isempty(fl)
        count = count + 1;
        seq(count) = uphalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(1,col) = 0;
        else
            tmpmat(1,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
    end
end
end
% endbulge is coded on the upper half
% go backwards from 3' side to 5' side
endbulge = zeros(size(bulge1));

```

```

lwhalf = structure(3:4,:);
pos = length(bulge1);
while bulge1(pos) == 1
    endbulge(pos) = 1;
    bulge1(pos) = 0;
    pos = pos - 1;
end
%lower half
bulge_row = 2; % 4 th line on structure is 2 line on lower half
bulge_row_opposite = 1;
[j,k] = find(isletter(lwhalf));
max_col = max(k);
for col = max_col:-1:1
    fl = find(isletter(lwhalf(:,col)));
    if ~isempty(fl)
        count = count + 1;
        seq(count) = lwhalf(fl,col);
        bulge = (fl == bulge_row);
        if(bulge)
            tmpmat(2,col) = 0;
        else
            tmpmat(2,col) = count;
        end
        bulge1(count) = 0;
        bulge2(count) = 0;
        if bulge & isletter(structure(bulge_row_opposite,col))
            bulge2(count) = 1;
        elseif bulge & ~isletter(structure(bulge_row_opposite,col))
            bulge1(count) = 1;
        end
        endbulge(count) = 0;
    end
end
anti_ind = zeros(size(bulge1));
for col=1:max_col
    if(tmpmat(1,col))
        anti_ind(tmpmat(1,col)) = tmpmat(2,col);
        anti_ind(tmpmat(2,col)) = tmpmat(1,col);
    end
end
return
function run_firstkpp(infile, outfile)
%run_firstkpp(infile, outfile)
model_filename = 'model_hmdcc440_params1.mat';
fitfile = 'fitfile_hmdcc440_params1_mfold5_proto5.mat';
fidin = fopen(infile,'r');
fidout = fopen(outfile,'a');
seqstot = 1000; %number of sequences to classify each loop
load(model_filename);
while ~feof(fidin)

```

```

disp('reading structure...');
[palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
    read_structure_with_id_fid(fidin,seqstot);
mfes = anti_inds_to_mfe(anti_inds);
[pos_est,score,edist_score,win_score] = ...
    firstkpp_predict_combined(model,palseq,anti_inds,bulges1,bulges2,endbulges);
[yside, yprec2] = interpolate_prob_new(score, fitfile);
res = [pal_id; pos_est; score; yprec2; edist_score; win_score];
fprintf(fidout, '%d %d %g %g %g %g\n', res);
end
fclose(fidin);
fclose(fidout);
param_file='params1'; params1;
model = model_params;
model.param_file = param_file;
set_name = model_params.trained_on;
fid = fopen(['zucker_draw_' set_name '.txt'],'r');
[palseq,anti_inds,bulges1,bulges2,endbulges,pal_id,energy,all_pal_ids] = ...
    read_structure_with_id_fid(fid,1000);
fclose(fid);
if(length(pal_id)~=length(all_pal_ids))
    error('in training data do not allow faulty seqs, take out of there');
end
mfes = anti_inds_to_mfe(anti_inds);
fname = ['mirseq_' set_name '.txt'];
[mirseq,mirlen] = read_seq_with_id(fname);
mirpos = locate_dicer(mirseq,palseq);
extension = [set_name '_params1'];
maxd = 5;
mfold = 5;
extension_proto = [set_name '_params1_mfold5_proto5'];
randstate = 1;
extension_random = [set_name '_params1_mfold5_randstate1'];
disp('building model from all data and saving it....')
% learn model , and add all known mirs to it
model = bayes_learn_win(palseq,anti_inds,bulges1,bulges2,endbulges,mirpos,mirlen,model);
% take the first ktup nucleotides of every miR
for i = 1:length(mirseq); mirseq{i} = mirseq{i}(1:model.ktup); end
model.seqs_d = transform_format(mirseq);
eval(['save model_' extension '.mat model']);
%%%%%%%%%%%%%
%%%%%%%%%
%%%%%%%%% random mfold %%%%%%%%%%
if(1)
disp('doing random mfold cv....')
[pos_est,score,edist_score,win_score] = mfold_cv_random(mirseq,mirpos,mirlen,palseq,anti_inds,...
    bulges1,bulges2,endbulges,mfold,randstate,model_params,1);
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est,score,mirpos,endbulges);

```

```

a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)
if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
eval(['print -djpeg ' extension_random '.jpeg']);
eval(['save fitfile_' extension_random '.mat xs ys xp2 yp2']);
figure;
fid = fopen(['info_and_criteria_' extension_random '.txt'],'w');
thresh_vec = [0:0.01:1];
clf;[thresh,acc2,captures] = analyse_errors_thresh_B(pos_est,score,mirpos,endbulges,thresh_vec);
grid
legend('off')
fprintf(fid,'%%thresh\tacc2\tcaptures\r\n');
for i=1:length(thresh)
    fprintf(fid,'%1.4f\t%1.4f\t%d\r\n',thresh(i),acc2(i),captures(i));
end
fclose(fid);
%save mfold results for each pal individually
fitfile = ['fitfile_' extension_random];
[yside,yprec2] = interpolate_prob_new(score, fitfile);
fid = fopen(['all_pal_res_' extension_random '.txt'],'w');
fprintf(fid,'%%pal_id\treal_mirpos\tfirstkpp_pos\tfirstkpp_score\typrec2\tfirstkpp_edist_score\tfirstk++_win_score\r\n');
fprintf(fid,'%%-----\r\n');
palres = [pal_id; mirpos; pos_est; score; yprec2; edist_score; win_score];
fprintf(fid, '%d %d %d %g %g %g %g\r\n', palres);
fclose(fid);
end
%%%%%%%%%%%%%%
%%%%%%%%%%%%%%
%%%%%%%%%%%%%% memebbers mfold %%%%%%%%%%
if(1)
disp('doing proto cv....')
filename =['clust_proto_members_' num2str(maxd) '_' set_name '.txt'];
clust_num = load(filename);
if length(clust_num) ~= length(palseq)
    error('clust_num wrong size');
end
[pos_est,score,edist_score,win_score] = mfold_cv_members(mirseq,mirpos,mirlen,palseq,anti_inds,...
    bulges1,bulges2,endbulges,clust_num,mfold,model_params);
figure
subplot(2,1,1)
res = analyse_errors_perc(pos_est,score,mirpos,endbulges);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
subplot(2,1,2)

```

```

if(~exist('num_bins'))
    num_bins = 6;
end
[xs,ys,xp2,yp2] = analyse_errors_bins2(pos_est,score,mirpos,endbulges,num_bins);
a=axis; a(3)=0; a(4)=1; axis(a); grid;
legend('off')
eval(['print -djpeg ' extension_proto '.jpeg']);
eval(['save fitfile_ ' extension_proto '.mat xs ys xp2 yp2']);
figure;
fid = fopen(['info_and_criteria_ ' extension_proto '.txt'],'w');
thresh_vec = [0:0.01:1];
clf;[thresh,acc2,captures] = analyse_errors_thresh_B(pos_est,score,mirpos,endbulges,thresh_vec);
grid
legend('off')
fprintf(fid,'%%thresh\tacc2\tcaptures\r\n');
for i=1:length(thresh)
    fprintf(fid,'%1.4f\t%1.4f\t%d\r\n',thresh(i),acc2(i),captures(i));
end
fclose(fid);
%save mfold results for each pal individually
fitfile = ['fitfile_ ' extension_proto];
[yside, yprec2] = interpolate_prob_new(score, fitfile);
fid = fopen(['all_pal_res_ ' extension_proto '.txt'],'w');
fprintf(fid,'%%pal_id\treal_mirpos\tfirstkpp_pos\tfirstkpp_score\typrec2\tfirstkpp_edist_score\tfirstk++_win_score\r\n');
fprintf(fid,'%%-----\r\n');
palres = [pal_id; mirpos; pos_est; score; yprec2; edist_score; win_score];
fprintf(fid, '%d %d %d %g %g %g %g\r\n', palres);
fclose(fid);
end
function seqs = transform_format(seqs,format);
%seqs = transform_format(seqs,format);
% format is either 'int' or 'nuc'
%if format not given, toggle format from int<-> nuc
% note that assume all seqs are in same format initially
if(nargin==1)
    if all(isletter(seqs{1}))
        format = 'int';
    else
        format = 'nuc';
    end
end
end
if(strcmp(format,'nuc'))
for i = 1:length(seqs)
    seqs{i} = int2nuc(seqs{i});
end
elseif(strcmp(format,'int'))
for i = 1:length(seqs)
    seqs{i} = nuc2int(seqs{i});
end
end

```

```

else
    error('transform_format: format (if given) must be int or nuc');
end
return

function [p_bp_arm5,p_bp_arm3] = win_base_pair_model_list(mfes,anti_inds,seqs,model,wps)
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(anti_inds) | numseqs~=length(seqs))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
win_len = model.ds_win_len;
base_pair_states = model.win_base_pair_states;
c_bp_arm5 = zeros(1,base_pair_states);
c_bp_arm3 = zeros(1,base_pair_states);
seqsbp = nuc2bp(seqs,anti_inds,base_pair_states);
for i = 1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    ai = anti_inds{i};
    is_paired = (ai~=0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
        for j = 1:base_pair_states
            c_bp_arm5(j) = c_bp_arm5(j)+sum(seqsbp{i}(pos5_on_arm5:pos3_on_arm5) == j);
            c_bp_arm3(j) = c_bp_arm3(j)+sum(seqsbp{i}(pos5_on_arm3:pos3_on_arm3) == j);
        end
    end
end
p_bp_arm5 = c_bp_arm5/sum(c_bp_arm5);
p_bp_arm3 = c_bp_arm3/sum(c_bp_arm3);
function [pb_arm5,pb_arm3,pb1_arm5,pb1_arm3,pb2_arm5,pb2_arm3] = ...
    win_bulge_pos_model_list(mfes,bulges1,bulges2,model,wps)
% on both sides of window from loop end of window
% pb1 - for bulges1 pb2 - for bulges2 pb - for total
win_len = model.ds_win_len;
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(bulges1) | numseqs~=length(bulges2))
    error('number of seqs differs from length(wps)');
end

```



```

% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
for i=1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    bulges{i} = bulges1{i}+bulges2{i};
    inds5_i = cell(0);
    inds3_i = cell(0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(bulges{i}),pos5_on_arm3+win_len-1);
        inds5_i{k} = pos3_on_arm5:-1:pos5_on_arm5; % always start from loop side
        inds3_i{k} = pos5_on_arm3:pos3_on_arm3;
    end
    inds5{i} = inds5_i;
    inds3{i} = inds3_i;
end
pb_arm5 = bulge_positional_list(model,bulges,inds5);
pb_arm3 = bulge_positional_list(model,bulges,inds3);
pb1_arm5 = bulge_positional_list(model,bulges1,inds5);
pb1_arm3 = bulge_positional_list(model,bulges1,inds3);
pb2_arm5 = bulge_positional_list(model,bulges2,inds5);
pb2_arm3 = bulge_positional_list(model,bulges2,inds3);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function p = bulge_positional_list(model,bulges,inds)
win_len = model.ds_win_len;
c = zeros(win_len,2);
p = zeros(win_len,1);
for i = 1:length(bulges)
    bulgesi = bulges{i};
    for k = 1:length(inds{i})
        this_inds = inds{i}{k};
        for j=1:length(this_inds)
            this_ind = this_inds(j);
            c(j,1) = c(j,1) + bulgesi(this_ind);
            c(j,2) = c(j,2) + (1-bulgesi(this_ind));
        end
    end
end
for j = 1:win_len
    p(j) = c(j,1)/sum(c(j,:));
end

```

```

end
function pos_scorei = win_score_2stagei(model,seqsi,anti_indsi,bulges1i,bulges2i,endbulgesi)
%function pos_scorei = win_score_2stagei(model,seqsi,anti_indsi,bulges1i,bulges2i,endbulgesi);
% pos_score is a vector having the length of the ith pal. pos_scorei(j) is the
% score of the window which gives that position of the pal. The entry is
% NULL if no window produces that pos5 or if it is on a loop. Note that each
% double stranded window gives two pos5, one on each arm, and they both have the same
% score - that of the ds_win.
mfe_i = anti_inds_to_mfe(anti_indsi);
pos_scorei = get_pos_scores(model,seqsi,mfe_i,anti_indsi,bulges1i,bulges2i,endbulgesi);
return
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function pos_scores = get_pos_scores(model,seqsi,mfe_i,ai,bulges1i,bulges2i, endbulgesi);
pos_scores = nan * ones(1,length(seqsi)); % initially all nan
p_mir = ones(1,size(mfe_i,1));
p_nonmir = ones(1,size(mfe_i,1));
wp_scores = nan * ones(1,size(mfe_i,1)); % in base pairs
if(model.win_use_loopdist)
    p_loopdist = loopdist_bp_prob_normal(model,mfe_i);
    p_mir = p_mir.*p_loopdist;
    p_nonmir = p_nonmir.*(1-p_loopdist);
end
if(model.win_use_num_bps)
    [p_num_bps_mir,p_num_bps_nonmir] = num_bps_prob_hist(model,mfe_i,ai);
    p_mir = p_mir.*p_num_bps_mir;
    p_nonmir = p_nonmir.*p_num_bps_nonmir;
end
if(model.win_use_win_sym)
    [p_win_sym_mir,p_win_sym_nonmir] = win_sym_prob(model,mfe_i,ai);
    p_mir = p_mir.*p_win_sym_mir;
    p_nonmir = p_nonmir.*p_win_sym_nonmir;
end
if(model.win_use_pos_bulge)
    [p_pos_bulge_mir,p_pos_bulge_nonmir] = win_bulges_pos_prob(model,mfe_i,bulges1i,bulges2i,0);
    p_mir = p_mir.*p_pos_bulge_mir;
    p_nonmir = p_nonmir.*p_pos_bulge_nonmir;
end
if(model.win_use_base_pair)
    [p_base_pair_mir,p_base_pair_nonmir] = win_base_pair_prob(model,mfe_i,ai,seqsi);
    p_mir = p_mir.*p_base_pair_mir;
    p_nonmir = p_nonmir.*p_base_pair_nonmir;
end
I = find((p_mir + p_nonmir) > 0);
wp_scores(I) = p_mir(I)./(p_mir(I)+p_nonmir(I));
% now transfer each of the win scores to the positions scores
for wp=1:length(wp_scores)
    s = wp_scores(wp);
    if(~isnan(s))
        pos3_on_arm5 = mfe_i(wp,1);
    end
end

```

```

pos5_on_arm3 = mfe(wp,2);
pos5_on_arm5 = max(1,pos3_on_arm5-model.ds_win_len+1);
pos_scores(pos5_on_arm3) = s;
pos_scores(pos5_on_arm5) = s;
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function p_loopdist = loopdist_bp_prob_normal(model,mfe);
n_bps = size(mfe,1);
wp = 1:n_bps;
zloopdist = ((n_bps - wp) - model.mean_loopdist_bp)/model.std_loopdist_bp;
p_loopdist = exp(-0.5*zloopdist.^2);
p_loopdist = p_loopdist/sum(p_loopdist);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_num_bps_mir,p_num_bps_nonmir] = num_bps_prob_hist(model,mfe,ai);
win_len = model.ds_win_len;
n_bps = size(mfe,1);
p_num_bps_mir = zeros(1,n_bps);
p_num_bps_nonmir = zeros(1,n_bps);
is_paired = (ai~=0);
for wp = 1:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
    win5inds = pos5_on_arm5:pos3_on_arm5;
    win3inds = pos5_on_arm3:pos3_on_arm3;
    if((length(win5inds)>=model.min_win_len) & (length(win3inds)>=model.min_win_len))
        numpaired5 = sum(is_paired(win5inds));
        numpaired3 = sum(is_paired(win3inds));
        num_bps_i = min(numpaired5,numpaired3);
        % mir
        tt = find(model.win_num_bps_mir_vals == num_bps_i);
        if(tt)
            p_num_bps_mir_i = model.win_num_bps_mir_ps(tt);
        else
            p_num_bps_mir_i = 0;
        end
        p_num_bps_mir_i = p_num_bps_mir_i*(win_len/mean(length(win5inds),length(win3inds)));
        p_num_bps_mir(wp) = p_num_bps_mir_i;
        % nonmir
        tt = find(model.win_num_bps_nonmir_vals == num_bps_i);
        if(tt)
            p_num_bps_nonmir_i = model.win_num_bps_nonmir_ps(tt);
        else
            p_num_bps_nonmir_i = 0;
        end
        p_num_bps_nonmir_i = p_num_bps_nonmir_i*(win_len/mean(length(win5inds),length(win3inds)));
    end
end

```

```

    p_num_bps_nonmir(wp) = p_num_bps_nonmir_i;
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_win_sym_mir,p_win_sym_nonmir] = win_sym_prob(model,mfe,ai);
win_len = model.ds_win_len;
n_bps = size(mfe,1);
p_win_sym_mir = zeros(1,n_bps);
p_win_sym_nonmir = zeros(1,n_bps);
is_paired = (ai~=0);
for wp = 1:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
    win5inds = pos5_on_arm5:pos3_on_arm5;
    win3inds = pos5_on_arm3:pos3_on_arm3;
    if((length(win5inds)>=model.min_win_len) & (length(win3inds)>=model.min_win_len))
        numunpaired5 = sum(~is_paired(win5inds));
        numunpaired3 = sum(~is_paired(win3inds));
        win_sym_i = abs(numunpaired5-numunpaired3);
        % mir
        tt = find(model.win_sym_mir_vals == win_sym_i);
        if(tt)
            p_win_sym_mir_i = model.win_sym_mir_ps(tt);
        else
            p_win_sym_mir_i = 0;
        end
        p_win_sym_mir_i = p_win_sym_mir_i*sqrt(win_len/mean(length(win5inds),length(win3inds)));
        p_win_sym_mir(wp) = p_win_sym_mir_i;
        % nonmir
        tt = find(model.win_sym_nonmir_vals == win_sym_i);
        if(tt)
            p_win_sym_nonmir_i = model.win_sym_nonmir_ps(tt);
        else
            p_win_sym_nonmir_i = 0;
        end
        p_win_sym_nonmir_i = p_win_sym_nonmir_i*sqrt(win_len/mean(length(win5inds),length(win3inds)));
        p_win_sym_nonmir(wp) = p_win_sym_nonmir_i;
    end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_pos_bulge_mir,p_pos_bulge_nonmir] = win_bulges_pos_prob(model,mfe,bulges1i,bulges2i,use_avg);
bulge_flag = model.win_bulge;
win_len = model.ds_win_len;
n_bps = size(mfe,1);
p_pos_bulge_mir = zeros(1,n_bps);
p_pos_bulge_nonmir = zeros(1,n_bps);

```

```

pb_arm5_mir = model.win_bulge_posit_arm5_mir;
pb_arm3_mir = model.win_bulge_posit_arm3_mir;
pb1_arm5_mir = model.win_bulge1_posit_arm5_mir;
pb1_arm3_mir = model.win_bulge1_posit_arm3_mir;
pb2_arm5_mir = model.win_bulge2_posit_arm5_mir;
pb2_arm3_mir = model.win_bulge2_posit_arm3_mir;
pb_arm5_nonmir = model.win_bulge_posit_arm5_nonmir;
pb_arm3_nonmir = model.win_bulge_posit_arm3_nonmir;
pb1_arm5_nonmir = model.win_bulge1_posit_arm5_nonmir;
pb1_arm3_nonmir = model.win_bulge1_posit_arm3_nonmir;
pb2_arm5_nonmir = model.win_bulge2_posit_arm5_nonmir;
pb2_arm3_nonmir = model.win_bulge2_posit_arm3_nonmir;
if(use_avg)
    pb_mir = 0.5*(pb_arm5_mir+pb_arm3_mir);
    pb_arm5_mir = pb_mir;
    pb_arm3_mir = pb_mir;
    pb1_mir = 0.5*(pb1_arm5_mir+pb1_arm3_mir);
    pb1_arm5_mir = pb1_mir;
    pb1_arm3_mir = pb1_mir;
    pb2_mir = 0.5*(pb2_arm5_mir+pb2_arm3_mir);
    pb2_arm5_mir = pb2_mir;
    pb2_arm3_mir = pb2_mir;
    pb_nonmir = 0.5*(pb_arm5_nonmir+pb_arm3_nonmir);
    pb_arm5_nonmir = pb_nonmir;
    pb_arm3_nonmir = pb_nonmir;
    pb1_nonmir = 0.5*(pb1_arm5_nonmir+pb1_arm3_nonmir);
    pb1_arm5_nonmir = pb1_nonmir;
    pb1_arm3_nonmir = pb1_nonmir;
    pb2_nonmir = 0.5*(pb2_arm5_nonmir+pb2_arm3_nonmir);
    pb2_arm5_nonmir = pb2_nonmir;
    pb2_arm3_nonmir = pb2_nonmir;
end
if(bulge_flag == 1)
    pb_arm5_mir = pb1_arm5_mir;
    pb_arm3_mir = pb1_arm3_mir;
    pb_arm5_nonmir = pb1_arm5_nonmir;
    pb_arm3_nonmir = pb1_arm3_nonmir;
    bulgesi = bulges1i;
elseif(bulge_flag == 2)
    pb_arm5_mir = pb2_arm5_mir;
    pb_arm3_mir = pb2_arm3_mir;
    pb_arm5_nonmir = pb2_arm5_nonmir;
    pb_arm3_nonmir = pb2_arm3_nonmir;
    bulgesi = bulges2i;
else
    % just use the total pb.
    bulgesi = bulges1i+bulges2i;
end
for wp = 1:n_bps
    pos3_on_arm5 = mfe(wp,1);

```

```

pos5_on_arm3 = mfe(wp,2);
pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
pos3_on_arm3 = min(length(bulgesi),pos5_on_arm3+win_len-1);
win5 = bulgesi(pos3_on_arm5:-1:pos5_on_arm5); % always start from loop side
win3 = bulgesi(pos5_on_arm3:pos3_on_arm3);
win5_len_actual = length(win5);
win3_len_actual = length(win3);
if((length(win5)>=model.min_win_len) & (length(win3)>=model.min_win_len))
    J0 = find(win5 == 0);
    J1 = find(win5);
    p_bulges5_mir_i = prod(pb_arm5_mir(J1)) * prod(1-pb_arm5_mir(J0));
    p_bulges5_mir_i = p_bulges5_mir_i^(win_len/win5_len_actual);
    p_bulges5_nonmir_i = prod(pb_arm5_nonmir(J1)) * prod(1-pb_arm5_nonmir(J0));
    p_bulges5_nonmir_i = p_bulges5_nonmir_i^(win_len/win5_len_actual);
    J0 = find(win3 == 0);
    J1 = find(win3);
    p_bulges3_mir_i = prod(pb_arm3_mir(J1)) * prod(1-pb_arm3_mir(J0));
    p_bulges3_mir_i = p_bulges3_mir_i^(win_len/win3_len_actual);
    p_bulges3_nonmir_i = prod(pb_arm3_nonmir(J1)) * prod(1-pb_arm3_nonmir(J0));
    p_bulges3_nonmir_i = p_bulges3_nonmir_i^(win_len/win3_len_actual);

    p_pos_bulge_mir(wp) = sqrt(p_bulges5_mir_i*p_bulges3_mir_i);
    p_pos_bulge_nonmir(wp) = sqrt(p_bulges5_nonmir_i*p_bulges3_nonmir_i);
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [p_base_pair_mir,p_base_pair_nonmir] = win_base_pair_prob(model,mfe,ai,seq);
win_len = model.ds_win_len;
base_pair_states = model.win_base_pair_states;
p_bp_arm5_mir = model.win_base_pair_arm5_mir;
p_bp_arm3_mir = model.win_base_pair_arm3_mir;
p_bp_arm5_nonmir = model.win_base_pair_arm5_nonmir;
p_bp_arm3_nonmir = model.win_base_pair_arm3_nonmir;
n_bps = size(mfe,1);
p_base_pair_mir = zeros(1,n_bps);
p_base_pair_nonmir = zeros(1,n_bps);
t1{1} = seq;
t2{1} = ai;
t3 = nuc2bp(t1,t2,base_pair_states);
seqbp = t3{1};
for wp = 1:n_bps
    pos3_on_arm5 = mfe(wp,1);
    pos5_on_arm3 = mfe(wp,2);
    pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
    pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
    win5inds = (pos5_on_arm5:pos3_on_arm5);
    win3inds = (pos5_on_arm3:pos3_on_arm3);
    if((length(win5inds)>=model.min_win_len) & (length(win3inds)>=model.min_win_len))
        % mir

```

```

p5_mir_i = 1;
p3_mir_i = 1;
for j = 1:base_pair_states
    p5_mir_i = p5_mir_i * p_bp_arm5_mir(j)^sum(seqbp(win5inds) == j);
    p3_mir_i = p3_mir_i * p_bp_arm3_mir(j)^sum(seqbp(win3inds) == j);
end
p5_mir_i = p5_mir_i.^(win_len/length(win5inds));
p3_mir_i = p3_mir_i.^(win_len/length(win3inds));
p_base_pair_mir(wp) = sqrt(p5_mir_i*p3_mir_i);
% nonmir
p5_nonmir_i = 1;
p3_nonmir_i = 1;
for j = 1:base_pair_states
    p5_nonmir_i = p5_nonmir_i * p_bp_arm5_nonmir(j)^sum(seqbp(win5inds) == j);
    p3_nonmir_i = p3_nonmir_i * p_bp_arm3_nonmir(j)^sum(seqbp(win3inds) == j);
end
p5_nonmir_i = p5_nonmir_i.^(win_len/length(win5inds));
p3_nonmir_i = p3_nonmir_i.^(win_len/length(win3inds));
p_base_pair_nonmir(wp) = sqrt(p5_nonmir_i*p3_nonmir_i);
end
end
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [win_sym_vals,win_sym_ps] = win_sym_model_list(mfes,anti_inds,model,wps)
numseqs = length(wps);
if(numseqs~=length(mfes) | numseqs~=length(anti_inds))
    error('number of seqs differs from length(wps)');
end
% transform wps into cell if it is not so.
if(~iscell(wps))
    for i=1:numseqs
        tt{i} = wps(i);
    end
    wps = tt;
end
beta = 0.5;
win_len = model.ds_win_len;
win_sym = [];
for i=1:numseqs
    wp_list = wps{i};
    mfe = mfes{i};
    ai = anti_inds{i};
    is_paired = (ai~=0);
    for k=1:length(wp_list)
        wp = wp_list(k);
        pos3_on_arm5 = mfe(wp,1);
        pos5_on_arm3 = mfe(wp,2);
        pos5_on_arm5 = max(1,pos3_on_arm5-win_len+1);
        pos3_on_arm3 = min(length(ai),pos5_on_arm3+win_len-1);
        numunpaired5 = sum(~is_paired(pos5_on_arm5:pos3_on_arm5));
    end
end

```

```
    numunpaired3 = sum(~is_paired(pos5_on_arm3:pos3_on_arm3));  
    win_sym = [win_sym,abs(numunpaired5-numunpaired3)];  
end  
end  
win_sym_vals = 0:model.win_num_bins_sym-1;  
n = hist(win_sym,win_sym_vals);  
n = n+beta;  
win_sym_ps = n/sum(n);  
%figure;bar(win_sym_vals,win_sym_ps);title('win sym training');
```